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# CRYSTALS OF THE ALPHA 1 BETA 1 INTEGRIN I-DOMAIN AND THEIR USE

# RELATED APPLICATIONS

This is a continuation of PCT/US99/23261, filed on October 6, 1999 as a continuation of prior U.S. provisional Serial number 60/103,301, filed October 6, 1998.

The entire disclosure of each of the aforesaid patent applications are incorporated herein by reference.

# **BACKGROUND OF THE INVENTION**

A major class of cell receptors that interacts with the constituents of the extracellular matrix (" ECM") (e.g, collagen, laminin) are the integrins which are transmembrane heterodimeric glycoproteins composed of noncovalently associated  $\alpha$  and  $\beta$  subunits. The integrin family contains at least  $16~\alpha$  subunits, seven of which contain an approximately 200 amino acid inserted domain in their N-terminal region variously called the "I-domain" or the "A-domain".

Processes such as cell differentiation, cell proliferation and cell migration in embryonic development, as well as remodeling and cell/tissue repair events, are dependent on communication of cells with the ECM. Alpha 1 beta 1 integrin (" $\alpha1\beta1$  integrin") is a cell-surface receptor for collagen I, collagen IV and laminin. It is also known as VLA-1. Indeed,  $\alpha1\beta1$  supports not only collagen-dependent adhesion and migration, but also is likely to be a critical collagen receptor on mesenchymally-derived cells that may be involved in ECM remodeling after injury (Gotwals et al.(1996), J. Clin. Invest. 97: p 2469-2477). The ability of cells to contract and organize collagen matrices is a critical component of any wound healing response. Improper regulation of  $\alpha1\beta1$  integrin may result in certain pathological conditions such as fibrosis.

Moreover, there is a limited, but provocative, literature suggesting that  $\alpha 1\beta 1$  may play a role in T cell/monocyte driven diseases. Anti- $\alpha 1\beta 1$  antibodies block T-cell dependent cytokine expression. Miyake et al., J. Exp. Med., 177: 863-868 (1993). Expression of  $\alpha 1\beta 1$  is upregulated in persistently activated, 2-4 week old cultured T cells (Hemler et al., Eur. J. Immunol., 15: 502-508 (1985)) and is also expressed on a high percentage of T cells isolated from the synovium of patients with rheumatoid arthritis. Hemler et al., J. Clin. Invest., 78: 696-702 (1986). Chronic tissue damage results from both

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resident activated T cells, and also monocytes/fibroblasts recruited by T cell-derived cytokines. Blocking the  $\alpha 1\beta 1$ -induced T cell interaction might relieve tissue damage by removing activated T cells and/or by diminishing inflammatory cytokine levels.

It would therefore be useful to design, identify or obtain potential drug candidates which would interfere with the  $\alpha 1\beta 1$  integrin-ECM or T-cell interaction(s). The recent emergence of drug design to identify candidates that play a role in a physiologically relevant biological pathway has provided a useful approach for obtaining, or designing, lead compounds for drugs.

Generally, this approach requires selecting a protein target molecule which plays a role in a physiologically relevant biological pathway. Typically, once an inhibitor or agonist, natural or synthesized, is found for the target molecule, it is modified or optimized to produce a candidate with the desired properties.

In order to more efficiently design or modify a ligand, it is useful to have a three-dimensional structure for the bioactive conformation of a known ligand as it binds to the target protein molecule. Furthermore, it is valuable to understand the detailed interactions of the ligand with its target protein by examining the three-dimensional structure of the protein target in complex with its known ligand. This allows the artisan to preserve the critical interactions with the protein, while modifying candidate ligands to interact more precisely with the protein, resulting in better potency and specificity.

However, the three dimensional crystal structure of the protein target is frequently unavailable due to the significant effort required to obtain crystals of sufficient size and quality to provide accurate information regarding the structure. For example, it is time consuming and often difficult to express, purify and characterize a protein. Additionally, once the protein of sufficient purity is obtained, it must be crystallized to a size and quality which is useful for x-ray diffraction and subsequent structure solution. Thus, although crystal structures can provide a wealth of valuable information in the field of drug design and discovery, crystals of certain biologically relevant molecules such as  $\alpha 1\beta 1$  integrin, are not readily available to those skilled in the art.

Furthermore, although the amino acid sequence of a target protein, such as  $\alpha 1\beta 1$  integrin, is known, this sequence information does not allow an accurate prediction of the crystal structure of the protein. Nor does the sequence information afford an understanding

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of the structural, conformational and chemical interactions between a ligand such as  $\alpha 1\beta 1$  integrin and its target.

Thus, there is a need for a detailed knowledge of the crystalline three-dimensional structure of the extracellular domain of  $\alpha 1\beta 1$  integrin, to effectively design, screen or optimize compounds capable of interfering with the  $\alpha 1\beta 1$  integrin-ECM and/or T-cell interactions.

A soluble version of  $\alpha 1\beta 1$  integrin can be made from its extracellular region or fragments thereof. As used herein, the term " $\alpha 1\beta 1$  integrin" includes soluble  $\alpha 1\beta 1$  integrin polypeptides lacking transmembrane and intracellular regions, homologs and analogs of  $\alpha 1\beta 1$  integrin or derivatives thereof. Crystals of the  $\alpha 1$  chain of  $\alpha 1\beta 1$  integrin or fragments thereof of a size and quality such as described herein, would allow performance of x-ray diffraction studies and enable those skilled in the art to conduct studies relating to the binding properties of  $\alpha 1\beta 1$  integrin, as well as the binding properties of molecules or molecular complexes which may associate with  $\alpha 1\beta 1$  integrin or fragments thereof.

# **SUMMARY OF THE INVENTION**

Accordingly, the present invention is directed to crystals of the  $\alpha 1$  chain of  $\alpha 1\beta 1$  integrin or crystals of fragments of the  $\alpha 1$  chain, of sufficient size and quality to obtain useful information about the properties of  $\alpha 1\beta 1$  integrin and molecules or complexes which may associate with it. The claimed invention provides the three-dimensional crystal structure of the Cys143 to Ala340 fragment of the  $\alpha 1$  chain of  $\alpha 1\beta 1$  integrin, which can be used to identify binding sites to solve the structure of unknown crystals, to provide mutants having desirable binding properties, and ultimately, to design, characterize, or identify molecules or chemical entities capable of interfering with the interaction between collagen or other ligands and  $\alpha 1\beta 1$ .

Additional features and advantages of the invention will be set forth in the description which follows, and in part will be apparent from the description, or may be learned by practice of the invention. The objectives and other advantages of the invention will be realized and attained by the compositions and methods particularly pointed out in the written description and claims hereof, as well as in the appended drawings.

To achieve these and other advantages, and in accordance with the purpose of the invention, as embodied and broadly described herein, the invention relates to a crystal of  $\alpha 1\beta 1$  integrin. More particularly, the invention relates to a crystal formed by a functional

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fragment of the extracellular domain of the  $\alpha 1$  chain of  $\alpha 1\beta 1$  (Cys143-Ala340), wherein the crystal has cell constants a= 34.77Å, b= 85.92Å, c= 132.56Å,  $\alpha = \beta = \gamma = 90$ Å, and a space group of P2<sub>1</sub>2<sub>1</sub>2<sub>1</sub>, and equivalents of that crystal. The claimed crystals of  $\alpha 1\beta 1$  are substantially described by the structural coordinates identified in Table II. The claimed crystals in certain embodiments are characterized by a binding site moiety comprising Asp154, Ser156, Asn157,Ser158, Leu222, Gln223, Thr224, Asp257, Glu259, His261, His288, Tyr289, Gly292, Leu294 and Lys298. Mutants, homologs, co-complexes and fragments of the claimed crystals are also contemplated herein.

The claimed invention in certain embodiments relates to heavy atom derivatives of the crystallized form of  $\alpha 1\beta 1$  integrin (143-340), and, more specifically, the heavy atom derivatives of the crystallized form of  $\alpha 1\beta 1$  described above. In various embodiments, the claimed invention relates to methods of preparing crystalline forms of  $\alpha 1\beta 1$ , or fragments thereof, by providing an aqueous solution comprising at least a fragment of  $\alpha 1\beta 1$ , providing a reservoir solution comprising a precipitating agent, mixing a volume of the al \( \text{1} \) solution with a volume of the reservoir solution and crystallizing the resultant mixed volume. In certain embodiments, the crystal is derived from an aqueous solution comprising the  $\alpha 1$  chain of  $\alpha 1\beta 1$  (Cys143-Ala340). In various embodiments, the concentration of  $\alpha 1\beta 1$  in the aqueous solution is about 1 to about 50 mg/ml, preferably about 5 mg/ml to about 15 mg/ml, and most preferably, about 10 mg/ml. The precipitating agents used in the invention may be any precipitating agent known in the art, preferably one selected from the group consisting of sodium citrate, ammonium sulfate and polyethylene glycol. Any concentration of precipitating agent may be used in the reservoir solution, however it is preferred that the concentration be about 20% weight per volume ("w/v") to about 50% w/v, more preferably about 25% w/v. Similarly, the pH of the reservoir solution may be varied, preferably between about 4 to about 10, most preferably about 6.5.

Various methods of crystallization can be used in the claimed invention, including, but not limited to, vapor diffusion, batch, liquid bridge, or dialysis. Vapor diffusion crystallization is preferred.

Additionally, the claimed invention relates to methods of using the claimed crystal, and the structural coordinates, in methods for screening, designing, or optimizing molecules or other chemical entities that may interfere with the interaction between  $\alpha 1\beta 1$ 

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ligands such as members of the extracellular matrix (e.g., collagen) and  $\alpha 1\beta 1$ . Thus, the structural coordinates of  $\alpha 1\beta 1$  or portions thereof can be used to solve the crystal structure of a mutant, homologue or co-complex of  $\alpha 1\beta 1$  or a fragment thereof, as well as to solve other unknown crystals which associate with  $\alpha 1\beta 1$  or fragments thereof.

In some embodiments, the structural coordinates of the  $\alpha 1$  chain of  $\alpha 1\beta 1$  (as exemplified in Table II) can be used to evaluate a chemical entity to obtain information about the binding of the chemical entity to  $\alpha 1\beta 1$ . The structural coordinates can be used to characterize chemical entities which interfere with the relationship between the extracellular matrix (i.e., collagen or laminin) and  $\alpha 1\beta 1$  such as inhibitors or agonists. The coordinates can also be used to optimize binding characteristics, to determine the orientation of ligands in a binding site of  $\alpha 1\beta 1$ . One skilled in the art will appreciate the numerous uses of the claimed invention in the areas of drug design, screening and optimization of drug candidates, as well as in determining additional unknown crystal structures.

In various embodiments, the claimed invention relates to a machine readable data storage medium having a data storage material encoded with machine readable data, which, when read by an appropriate machine, can display a three dimensional representation of a crystal. The crystals displayed comprise a fragment of  $\alpha1\beta1$  such as that described by the coordinates in Table II, or a crystal having a binding site moiety comprising amino acids Asp154, Ser156, Asn157,Leu222, Gln223, Thr224, Asp257, Glu259, His261, His288, Tyr289, Gly292, Leu294 and Lys298.

In other embodiments, the claimed invention relates to a method for determining a at least a portion of a three dimensional structure of a chemical entity or molecular complex by calculating phases from the structural coordinates of a crystal of a fragment of  $\alpha 1\beta 1$ , calculating the electron density map from the phases obtained, and then determining at least a portion of the unknown structure based upon the electron density map.

In yet other embodiments, the invention relates to methods for evaluating the ability of a chemical entity to associate with  $\alpha 1\beta 1$ . The methods employ computational or experimental means to perform a fitting operation between the chemical entity and the  $\alpha 1\beta 1$  to obtain data related to the association, and analyzing the data to determine the characteristics. Chemical entities identified by these methods which are capable of interfering with the in vivo or in vitro association between the extracellular matrix and

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 $\alpha 1\beta 1$  are also encompassed by the claimed invention. The claimed chemical entities may comprise binding sites substantially similar to those of  $\alpha 1\beta 1$ , or, alternatively may comprise binding sites capable of associating with the binding sites of  $\alpha 1\beta 1$ .

It is to be understood that both the foregoing general description and the following detailed description are exemplary and explanatory and are intended to provide further explanation of the invention as claimed.

The accompanying drawings are included to provide a further understanding of the invention and are incorporated in and constitute a part of this specification, illustrate several embodiments of the invention, and together with the description, serve to explain the principles of the invention.

#### **BRIEF DESCRIPTION OF THE FIGURES**

Figure 1: 2Fo-Fc electron density map for a representative region of the  $\alpha 1$  I-domain crystal structure, contoured at 1Sigma.

Figure 2: Ribbon representation of the fold of the  $\alpha 1$  I-domain molecule. The arrow points to the MIDAS binding site.

#### DETAILED DESCRIPTION OF THE INVENTION

In order that the invention described herein may be more fully understood, the following detailed description is set forth.

The present invention relates to a crystal of a soluble fragment of the extracellular domain of the  $\alpha 1\beta 1$  integrin. Specifically, it relates to a crystal of a soluble protein comprising the sequence from Cys143 to Ala340 of the  $\alpha 1$  chain of  $\alpha 1\beta 1$  integrin ("s $\alpha 1\beta 1(143-340)$ "), the structure of s $\alpha 1\beta 1(143-340)$  as determined by X-ray crystallography, and the use of the s $\alpha 1\beta 1(143-340)$  structure and that of its homologs, mutants and co-complexes to design, identify, characterize, screen and/or optimize candidate inhibitors or agonists of  $\alpha 1\beta 1$  activity.

# A. **DEFINITIONS**

The term  $\alpha 1\beta 1$  integrin ("VLA-1" or " $\alpha 1\beta 1$ " or " $\alpha 1\beta 1$ " integrin", used interchangeably) herein refers to a genus of polypeptides which are capable of binding to members of the extracellular matrix proteins such as laminin or collagen, or homologs or fragments thereof. The term as used herein includes  $s\alpha 1\beta 1$  integrin 143-340), homologs, mutants, equivalents and fragments thereof.

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The term "co-complex" refers to an  $\alpha 1\beta 1$  or a mutant or homolog of  $\alpha 1\beta 1$  in covalent or non-covalent association with a chemical entity.

The term "homolog" or "homologous"- as used herein is synonymous with the term "identity" and refers to the sequence similarity between two polypeptides, molecules or between two nucleic acids. When a position in both of the two compared sequences is occupied by the same base or amino acid monomer subunit (for instance, if a position in each of the two DNA molecules is occupied by adenine, or a position in each of two polypeptides is occupied by a lysine), then the respective molecules are homologous at that position. The percentage homology between two sequences is a function of the number of matching or homologous positions shared by the two sequences divided by the number of positions compared x 100. For instance, if 6 of 10 of the positions in two sequences are matched or are homologous, then the two sequences are 60% homologous. By way of example, the DNA sequences CTGACT and CAGGTT share 50% homology (3 of the 6 total positions are matched). Generally, a comparison is made when two sequences are aligned to give maximum homology. Such alignment can be provided using, for instance, the method of Needleman et al., J. Mol Biol. 48: 443-453 (1970), implemented conveniently by computer programs such as the Align program (DNAstar, Inc.). Homologous sequences share identical or similar amino acid residues, where similar residues are conservative substitutions for, or "allowed point mutations" of, corresponding amino acid residues in an aligned reference sequence. In this regard, a "conservative substitution" of a residue in a reference sequence are those substitutions that are physically or functionally similar to the corresponding reference residues, e.g., that have a similar size, shape, electric charge, chemical properties, including the ability to form covalent or hydrogen bonds, or the like. Particularly preferred conservative substitutions are those fulfilling the criteria defined for an "accepted point mutation" in Dayhoff et al., 5: Atlas of Protein Sequence and Structure, 5: Suppl. 3, chapter 22: 354-352, Nat. Biomed. Res. Foundation, Washington, D.C. (1978).

The term "mutant" refers to an  $\alpha 1\beta 1$  integrin or fragment thereof, characterized by the replacement, deletion, or insertion of at least one amino acid from the wild-type. Such a mutant may be prepared, for example, by expression of  $\alpha 1\beta 1$  integrin previously altered in its coding sequence by oligonucleotide-directed mutagenesis.

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The term "positively charged amino acid" includes any amino acid, natural or unnatural, having a positively charged side chain under normal physiological conditions. Examples of positively charged naturally occurring amino acids are arginine, lysine and histidine.

The term "negatively charged amino acid" includes any amino acid, natural or unnatural, having a negatively charged side chain under normal physiological conditions. Examples of negatively charged naturally occurring amino acids are aspartic acid and glutamic acid.

The term "hydrophobic amino acid" means any amino acid having an uncharged, nonpolar side chain that is relatively insoluble in water. Examples are alanine, leucine, isoleucine, valine, proline, phenylalanine, tryptophane and methionine.

The term "hydrophilic amino acid" means any amino acid having an uncharged, polar side chain that is relatively soluble in water. Examples are serine, threonine, tyrosine, asparagine, glutamine, and cysteine.

The term "altered surface charge" means a change in one or more of the charge units of a mutant polypeptide, at physiological pH, as compared to  $\alpha 1\beta 1$  integrin. The change in surface charge can be determined by measuring the isoelectric point (pI) of the polypeptide molecule containing the substituted amino acid and comparing it to the pI of the wild-type molecule.

The term "associating with" refers to a condition of proximity between two chemical entities, or portions thereof, for example, an  $\alpha 1\beta 1$  integrin or portions thereof and a chemical entity. The association may be non-covalent, wherein the juxtaposition is energetically favored by hydrogen bonding, van der Waals interaction, or electrostatic interaction, or it may be a covalent association.

The term "binding site" refers to any or all of the sites where a chemical entity binds or associates with another entity.

The term "structural coordinates" refers to the coordinates derived from mathematical equations related to the patterns obtained on diffraction of a monochromatic beam of X-rays by the atoms (scattering centers) of molecule in crystal form. The diffraction data are used to calculate an electron density map of the repeating units of the crystal. Those skilled in the art will understand that the data obtained are dependent upon the particular system used, and hence, different coordinates may in fact describe the same

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crystal if such coordinates define substantially the same relationship as those described herein. The electron density maps are used to establish the positions of the individual atoms within the unit cell of the crystal.

Those of skill in the art understand that a set of structural coordinates determined by X-ray crystallography is not without standard error. Table II is the atomic coordinates of the I-domain of the  $\alpha$ 1 chain of  $\alpha$ 1 $\beta$ 1 integrin (143-340). For the purpose of this invention, any set of structural coordinates of  $\alpha$ 1 $\beta$ 1 (143-340) that have a root mean square deviation of equivalent protein backbone atoms of less than about 2Å when superimposed—using backbone atoms—on the structural coordinates in Table II shall be considered identical. Preferably the deviation is less than about 1Å and more preferably less than about 0.5Å.

The term "heavy atom derivatization" refers to a method of producing a chemically modified form of a crystallized  $\alpha 1\beta 1$  integrin. In practice, a crystal is soaked in a solution containing heavy metal atom salts, or organometallic compounds, e.g., lead chloride, gold thiomalate, thimerosal or uranyl acetate, which can diffuse through the crystal and bind to the surface of the protein. The location of the bound heavy metal atom(s) can be determined by X-ray diffraction analysis of the soaked crystal. This information can be used to generate the phase information used to construct the three-dimensional structure of the molecule.

The term "unit cell" refers to a basic shaped block. The entire volume of a crystal may be constructed by regular assembly of such blocks. Each unit cell comprises a complete representation of the unit of pattern, the repetition of which builds up the crystal.

The term "space group" refers to the arrangement of symmetry elements of a crystal.

The term "molecular replacement" refers to a method that involves generating a preliminary structural model of a crystal whose structural coordinates are unknown, by orienting and positioning a molecule whose structural coordinates are known e.g. the  $\alpha 1$  I-domain coordinates in Table II, within the unit cell of the unknown crystal, so as to best account for the observed diffraction pattern of the unknown crystal. Phases can then be calculated from this model, and combined with the observed amplitudes to give an approximate Fourier synthesis of the structure whose coordinates are unknown. This in turn can be subject to any of the several forms of refinement to provide a final accurate

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structure of the unknown crystal. See, e.g., Lattman, E., "Use of the Rotation and Translation Functions", Methods in Enzymology, 115, pp. 55-77 (1985); Rossman, ed., "The Molecular Replacement Method", Int. Sci. Rev. Ser. No. 13, Gordon and Breach, New York (1972), all specifically incorporated by reference herein. Using the structural coordinates provided by this invention, molecular replacement may be used to determine the structural coordinates of a crystalline co-complex, unknown ligand, mutant, homolog, or of a different crystalline form of  $\alpha 1\beta 1$  or fragment thereof. Additionally, the claimed crystal and its coordinates may be used to determine the structural coordinates of a chemical entity which associates with  $\alpha 1\beta 1$  or fragment or with a member of the extracellular matrix which is a ligand for  $\alpha 1\beta 1$  or fragment thereof.

The term "chemical entity" as used herein shall mean, for example, any molecule, molecular complex, compound or fragment thereof.

Mutants of  $\alpha 1\beta 1$  or fragments thereof may be generated by site-specific incorporation of natural or unnatural amino acids into  $\alpha 1\beta 1$  or fragments using general biosynthetic methods known to those skilled in the art. For example, the codon encoding the amino acid of interest in wild-type  $\alpha 1$  chain of  $\alpha 1\beta 1$  may be replaced by a "blank" nonsense codon, such as TAG, using oligonucleotide-directed mutagenesis. A suppressor tRNA directed against this codon can then be chemically aminoacylated in vitro with the desired amino acid. The aminoacylated tRNA can then be added to an in vitro translation system to yield a mutant  $\alpha 1\beta 1$  with the site-specific incorporated amino acid.

The term "soluble fragment" of α1β1 and any equivalent term used herein, refers to a functional fragment of α1β1, and more particularly refers to a functional α1 chain. The term "functional" as used in this context refers to a soluble fragment of the extracellular domain that is capable of binding to, or associating with a member of the extracellular matrix such as collagen or laminin or any fragments or homologs thereof, including molecular complexes comprising fragments thereof. Such binding may be demonstrated through immunoprecipitation experiments, using standard protocols known in the art.

# A. ALPHA 1 BETA 1 INTEGRIN, its Crystal, and its Biological Implications

It will be understood that throughout the specification and claims, the positional location of the amino acids described is not an absolute value, but rather, defines the relative relationship of the residues. Thus it is intended that the present invention encompass the sequences having the same or similar relative positions.

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For the first time, the present invention permits the use of molecular design techniques to design, screen and optimize chemical entities and compounds, including inhibitory compounds, capable of binding to the active site or accessory binding site of  $\alpha 1\beta 1$ , in whole or in part. The  $\alpha 1\beta 1$  integrin is a membrane-bound protein of considerable biomedical interest because of its involvement in important functions mediated by its binding to the extracellular matrix such as collagen. Since  $\alpha 1\beta 1$  is found in various vertebrate (e.g., mammalian) organisms, such as humans, mice, rats, and pigs, the claimed invention is not intended to be limited to any particular species or organism.

The  $\alpha 1\beta 1$  integrin (VLA-1)is a member of the integrin family of proteins. The crystal structure of I-domains from other members of this family,  $\alpha M$ ,  $\alpha L$  and  $\alpha 2$ , have been described. See Dickeson & Santoro (1998) Cell. Mol. Life Sci. 54, 556-566 for a review and Emsley et al., J. Biol.Chem. 272, 28512-28517.

These I-domains were used as a framework for understanding the  $s\alpha 1\beta 1$  integrin(143-340) crystal structure. However, despite certain similarities, the differences between the I-domain of  $\alpha 1$  and the I-domains of  $\alpha M$ ,  $\alpha L$ , and  $\alpha 2$  integrins, confirm that these ligand-receptor systems utilize spatially overlapping, but nonidentical and nonconserved sites of contact residues with different molecular determinants of binding.

Considering the complexity and overlap of the various integrins and their biological processes, the fact that  $\alpha 1\beta 1$  binds specifically to its ligand suggests that inhibiting  $\alpha 1\beta 1$  signaling may have important therapeutic applications. The crystal structure of  $s\alpha 1\beta 1$  (143-340) presented here is expected to be useful in the design, identification, characterization and optimization of such therapeutic agents.

The following detailed description of applicants invention encompasses the (a) crystal structure of the  $\alpha 1$  chain I-domain (Cys143-Ala340) of  $\alpha 1\beta 1$  integrin and the coordinates thereof, (b) the binding sites thereof, (c) methods of making an  $\alpha 1\beta 1$  crystal or fragment thereof, and (d) methods of using the  $\alpha 1\beta 1$  crystal or fragment thereof and its structural coordinates.

# (a) Crystal Structure of the α1 I-domain

The claimed invention provides crystals of  $\alpha 1\beta 1$  integrin as well as the structure derived therefrom. The crystals are derived from the  $\alpha 1$  I-domain of the rat. Nevertheless, the sequence identity between rat and human alpha 1 I-domains is about 95%. Specifically, the amino acids which differ between the rat and human  $\alpha 1$  I-domains are

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Ile166, Asn214, Gly217, Arg 218, Gln219 Leu222, Tyr262, Gln267, His288, Ala330 (rat I-domain sequence). Most of them are located a relatively long distance away from the metal-ion-dependent-adhesion-site (MIDAS) of the α1 I-domain, the site likely to be involved in ligand binding. The only 2 amino acids that are expected to participate in ligand binding are the Leu222 and His288. This high degree of primary amino acid sequence identity indicates that the 3-dimensional structures of rat and human 1 I-domains are expected to be similar. Therefore, we used the crystal structure of the rat 1 I-domain for the purposes discussed in this patent and we fully expect that the 3-dimensional structure of the human 1 I-domain will have substantially identical coordinates for the main chain atoms.

The claimed invention provides crystals of a fragment from the  $\alpha 1$  chain of  $\alpha 1\beta 1$  integrin(143-340) having unit cells which are rhombohedral, and having the following dimensions a= 34.77Å; b=85.92Å and c= 132.56Å;  $\alpha = \beta = \gamma = 90$ Å. Almost all of the residues of the I-domain of the  $\alpha 1$  chain of  $\alpha 1\beta 1$  integrin, except for residues 143-144 of the N terminus and 336-340 of the C-terminus, are well defined in the final electron density map shown in Figure 1. The current model consists of 386 amino acid residues and 199 water molecules with a crystallographic R factor of 23.5 % and an R<sub>free</sub> of 30.2% for data between 100Å and 2.2Å.

There are two copies of the molecule (termed "A" and "B") in the asymmetric unit. The Ramachandran diagram shows that 384 out of the 386 amino acid residues have  $(\phi,\psi)$  angles within the allowed regions. The exception is residue Glu192 (A & B). In the atomic coordinates of the rat I-domain crystal structure (Tabld II), residues Thr145, Gln146, Arg234 of molecule A and Thr145 and Arg175 of molecule B are modeled as alanines because of absence of electron density for the side chain. In addition, residues 143, 145, 337, 338, 339,340 of molecule A and 143, 144, 339, 340 of molecule B are not included in the model due to weak electron density.

The I-domain adopts the nucleotide-binding fold (Figure 2) characterized by the existence of seven helices surrounding a core of five parallel  $\beta$ -strands and one antiparallel  $\beta$ -strand. The dimensions of the molecule are 25Å x 30Å x 50Å. The overall fold is similar to that of  $\alpha M$ ,  $\alpha L$  and  $\alpha 2$  I-domains and in particular to that of the  $\alpha 2$  I-domain. By homology to the other I-domains it is inferred that the metal-ion-dependent-adhesion-site (MIDAS) of the  $\alpha 1$  I-domain consists of residues Asp154, Ser156, Ser158, Thr224, Asp

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257. The MIDAS site is the site of Mg or Mn cation binding and is expected to be involved in ligand binding. The crystals were grown in the absence of Mg or Mn cations (except for contaminants) and there is no electron density visible in that would correspond to a cation. The structure appears to have the "inactive" conformation according to the model proposed in Lee et al. (1995) Structure 3, 1333-1340. The conformations of molecules A and B are very similar.

# (b) Binding Sites

Modeling studies done for collagen binding on the α2 I-domain (Emsley et al. (1997) J. Biol.Chem. 272, 28512-28517) suggest that the binding site for collagen is expected to include the MIDAS site as well as several neighboring residues. By analogy, the binding site of the α1 I-domain for collagen is expected to include residues Asp154, Ser156, Asn157, Ser158, Leu222, Gln223, Thr224, Asp257, Glu259, His261, His288, Tyr289, Gly292, Leu294 and Lys298. Of interest is the observation that the MIDAS site of the α1 I-domain (molecule A in the crystal) forms an interaction with Arg246 of molecule B. It is possible that the positive charge of the arginine side chain replaces the positive charge of the missing metal ion.

#### (c) Methods of Making an α1β1 Crystal

In various embodiments, the claimed invention relates to methods of preparing crystalline forms of  $\alpha1\beta1$ , or fragments thereof by first providing an aqueous solution comprising  $\alpha1\beta1$  or a fragment of  $\alpha1\beta1$ . A reservoir solution comprising a precipitating agent is then mixed with a volume of the  $\alpha1\beta1$  solution and the resultant mixed volume is then crystallized. In certain embodiments, the crystal is derived from an aqueous solution comprising  $s\alpha1\beta1(127-340)$ . In preferred embodiments, the crystal is derived from an aqueous solution comprising  $s\alpha1\beta1(143-340)$ . The concentration of  $\alpha1\beta1$  or fragment in the aqueous solution may vary, and is preferably about 1 to about 50 mg/ml, more preferably about 5 mg/ml to about 15 mg/ml, and most preferably, about 10 mg/ml. Similarly, precipitating agents used in the invention may vary, and may be selected from any precipitating agent known in the art. Preferably the precipitating agent is selected from the group consisting of sodium citrate, ammonium sulfate and polyethylene glycol, with polyethylene glycol 8000 being most preferred. Any concentration of precipitating agent may be used in the reservoir solution, however it is preferred that the concentration be about 20% w/v to about 35%w/v, more preferably about 25% w/v. The pH of the

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reservoir solution may also be varied, preferably between about 4 to about 10, most preferably about 6.5. One skilled in the art will understand that each of these parameters can be varied without undue experimentation and acceptable crystals will still be obtained. In practice, once the appropriate precipitating agents, buffers or other experimental variables are determined for any given growth method, any of these methods or any other methods can be used to grow the claimed crystals. One skilled in the art can determine the variables depending upon his particular needs.

Various methods of crystallization can be used in the claimed invention, including, but not limited to, vapor diffusion, batch, liquid bridge, or dialysis. Vapor diffusion crystallization is preferred. See, e.g. McPherson et al., "Preparation and Analysis of Protein Crystals", Glick, Ed., pp 82-159, John Wiley & Co. (1982); Jancarik et.al., "Sparse matrix sampling: a screening method for crystallization of protein", J. Appl. Cryst. 24, 409-411 (1991), specifically incorporated by reference herein.

In vapor diffusion crystallization, a small volume (i.e. a few milliliters) of protein solution is mixed with a solution containing a precipitating agent. This mixed volume is suspended over a well containing a small amount, i.e. about 1 ml, of precipitating solution. Vapor diffusion from the drop to the well will result in crystal formation in the drop.

The dialysis method of crystallization utilizes a semipermeable size exclusion membrane which retains the protein but allows small molecules (i.e. buffers and precipitating agents) to diffuse in and out. In dialysis, rather than concentrating the protein and the precipitating agent by evaporation, the precipitating agent is allowed to slowly diffuse through the membrane and reduce the solubility of the protein while keeping the protein concentration fixed.

The batch methods generally involve the slow addition of a precipitating agent to an aqueous solution of protein until the solution just becomes turbid, at this point the container can be sealed and left undisturbed for a period of time until crystallization occurs.

Thus, applicants intend that the claimed invention encompass any and all methods of crystallization. One skilled in the art can choose any of such methods and vary the parameters such that the chosen method results in the desired crystals.

#### (d) Use of ALPHA 1 BETA 1 INTEGRIN Crystal and its Coordinates

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The claimed crystals, and coordinates describing them, permit the use of molecular design techniques to design, select and synthesize chemical entities and compounds, including inhibitory compounds or agonists capable of binding to, or associating with, the binding site of  $\alpha 1\beta 1$  integrin in whole or in part.

One approach enabled by this invention is the use of the structural coordinates defined herein to design chemical entities that bind to or associate with,  $\alpha 1\beta 1$  or fragments of  $\alpha 1\beta 1$  and alter the physical properties of the compounds in different ways. Thus, properties such as, for example, solubility, affinity, specificity, potency, on/off rates or other binding characteristics may all be altered and/or optimized.

One may design desired chemical entities by probing a crystal of the present invention with a library of different entities to determine optimal sites for interaction between candidate chemical entities and  $\alpha 1\beta 1$  or fragments of  $\alpha 1\beta 1$ . For example, high resolution x-ray diffraction data collected from crystals saturated with solvent allows the determination of where each type of solvent molecule sticks. Small molecules that bind tightly to those sites can then be designed and synthesized and tested for the desired activity. Once the desired activity is obtained, the molecules can be further optimized.

The claimed invention also makes it possible to computationally screen small molecule data bases or computationally design chemical entities or compounds that can bind in whole, or in part, to extracellular matrix proteins or  $\alpha 1\beta 1$  or fragments thereof. They may also be used to solve the crystal structure of mutants, co-complexes, or of the crystalline form of any other molecule homologous to, or capable of associating with, at least a portion of  $\alpha 1\beta 1$ , i.e., the I-domain of the  $\alpha 1$  chain.

One method that may be employed for this purpose is molecular replacement. An unknown crystal structure, which may be any unknown structure, such as, for example, another crystal form of  $\alpha 1\beta 1$ , an  $\alpha 1\beta 1$  mutant, or a co-complex with an extracellular matrix protein such as laminin or collagen, or any other unknown crystal of a chemical entity which associates with  $\alpha 1\beta 1$  or fragment which is of interest, may be determined using the structural coordinates of this invention, set forth in Table II. Co-complexes with  $\alpha 1\beta 1$  or fragments may include, but are not limited to, laminin- $\alpha 1\beta 1$ , collagen- $\alpha 1\beta 1$ , and "small molecule"- $\alpha 1\beta 1$ . This method will provide an accurate structural form for the unknown crystal more quickly and efficiently than attempting to determine such information without the claimed invention. The information obtained can thus be used to

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optimize potential inhibitors or agonists of  $\alpha 1\beta 1$ , and more importantly, to design and synthesize novel classes of chemical entities which will affect the relationship between  $\alpha 1\beta 1$  and its ligand(s) in the extracellular matrix.

The design of compounds that inhibit or agonize  $\alpha 1\beta 1$  according to this invention generally involves consideration of at least two factors. First, the compound must be capable of physically or structurally associating with  $\alpha 1\beta 1$  or a fragment thereof. The association may be any physical, structural, or chemical association, such as, for example, covalent or noncovalent bonding, van der Waals interactions, hydrophobic or electrostatic interactions.

Second, the compound must be able to assume a conformation that allows it to associate with  $\alpha 1\beta 1$  or fragment thereof. Although not all portions of the compound will necessarily participate in the association with  $\alpha 1\beta 1$  or fragment, those non-participating portions may still influence the overall conformation of the molecule. This in turn may have a significant impact on the desirability of the compound. Such conformational requirements include the overall three-dimensional structure and orientation of the chemical entity or compound in relation to all or a portion of the binding site.

The potential inhibitory or binding effect of a chemical compound on  $\alpha 1\beta 1$  or fragment may be analyzed prior to its actual synthesis and testing by the use of computer modeling techniques. If the theoretical structure of the given compound suggests insufficient interaction and association between it and  $\alpha 1\beta 1$  or its fragment(s), the need for synthesis and testing of the compound is obviated. However, if computer modeling indicates a strong interaction, the molecule may then be synthesized and tested for its ability to bind to  $\alpha 1\beta 1$  or fragment thereof. Thus, expensive and time consuming synthesis of inoperative compounds may be avoided.

An inhibitory or other binding compound of  $\alpha 1\beta 1$  or fragment may be computationally evaluated and designed by means of a series of steps in which chemical entities or fragments are screened and selected for their ability to associate with the individual binding sites of  $\alpha 1\beta 1$ .

Thus, one skilled in the art may use one of several methods to screen chemical entities or fragments for their ability to associate with  $\alpha 1\beta 1$  and more particularly, with the individual binding sites of the I-domain of the  $\alpha 1$  chain of  $\alpha 1\beta 1(143-340)$ . This process may begin by visual inspection of, for example, the binding site on a computer screen

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based on the coordinates in Table II. Selected fragments or chemical entities may then be positioned in a variety of orientations, or "docked", within an individual binding pocket of  $\alpha 1\beta 1$ . Docking may be accomplished using software such as Quanta and Sybyl, followed by energy minimization and molecular dynamics with standard molecular mechanics force fields, such as CHARMM and AMBER.

Specialized computer programs may be of use for selecting interesting fragments or chemical entities. (GRID, available from Oxford University, Oxford, UK; MCSS or CATALYST, available from Molecular Simulations, Burlington, MA; AUTODOCK, available from Scripps Research Institute, La Jolla, CA; DOCK available from University of California, San Francisco, CA., XSITE, University College of London, UK.)

Once suitable chemical entities or fragments have been selected, they can be assembled into an inhibitor or agonist. Assembly may be by visual inspection of the relationship of the fragments to each other on the three-dimensional image displayed on a computer screen, in relation to the structural coordinates disclosed herein.

Alternatively, one may design the desired chemical entities "de novo", experimentally, using either an empty binding site, or optionally including a portion of a molecule with desired activity. Thus, for example, one may use solid phase screening techniques where either  $\alpha 1\beta 1$  or a fragment thereof, or candidate chemical entities to be evaluated are attached to a solid phase thereby identifying potential binders for further study or optimization.

Basically, any molecular modeling techniques may be employed in accordance with the invention; these techniques are known, or readily available to those skilled in the art. It will be understood that the methods and compositions disclosed herein can be used to identify, design or characterize not only entities which will associate or bind to  $\alpha1\beta1$  or fragment thereof, but alternatively to identify, design or characterize entities which, like  $\alpha1\beta1$ , will bind to extracellular matrix proteins, thereby disrupting the  $\alpha1\beta1$ -ECM interaction. The claimed invention is intended to encompass these methods and compositions broadly.

Once a compound has been designed or selected by the above methods, the efficiency with which that compound may bind to  $\alpha 1\beta 1$  or fragment thereof may be tested and optimized using computational or experimental evaluation. Various parameters can be optimized depending on the desired result. These include, but are not limited to,

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specificity, affinity, on/off rates, hydrophobicity, solubility and other characteristics readily identifiable by the skilled artisan. Thus, one may optionally make substitutions, deletions, or insertions in some of the components of the chemical entities in order to improve or modify the binding properties. Generally, initial substitutions are conservative, i.e the replacement group will have approximately the same size, shape, hydrophobicity and charge as the original component.

The present invention also enables the design of mutants of  $\alpha 1\beta 1$  and the solving of their crystal structure. More particularly, the claimed invention enables one skilled in the art to determine the location of binding sites and interfaces, particularly in the I-domain of the  $\alpha 1$  chain, thereby identifying desirable sites for mutation.

For example, mutation may be directed to a particular site or combination of sites on the I-domain, by replacing or substituting one or more amino acid residues. Such mutants may have altered binding properties which may or may not be desirable.

The mutants may be prepared by any methods known in the art, such as for example, site directed mutagenesis, deletion or addition, and then tested for any properties of interest. For example, mutants may be screened for an altered charge at a particular pH, tighter binding, better specificity etc.

Additionally, the claimed invention is useful for the optimization of potential small molecule drug candidates. Thus, the claimed crystal structures can be also be used to obtain information about the crystal structures of complexes of the  $\alpha 1\beta 1$  integrin and small molecule inhibitors. For example, if the small molecule inhibitor is co-crystallized with  $\alpha 1\beta 1$  or a fragment thereof, then the crystal structure of the complex can be solved by molecular replacement using the known coordinates of  $\alpha 1\beta 1$  or fragment for the calculation of phases. Such information is useful, for example, for determining the nature of the interaction between the I-domain of  $\alpha 1\beta 1$  integrin and the small molecule inhibitor, and thus, may suggest modifications which would improve binding characteristics such as affinity, specificity and kinetics.

Example 1: <u>Determination of Crystal Structure of the ALPHA 1 INTEGRIN I-DOMAIN</u> (127-340)

30 A. Expression and purification of α1 integrin I-domain.

A soluble fragment of the extracellular domain of rat integrin  $\alpha 1\beta 1$   $\alpha 1$  chain containing amino acid residues Val127 to the C-terminal residue Ala340 was produced in

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soluble form and purified as follows: The gene encoding the rat  $\alpha 1\beta 1$  I-domain sequence of amino acids Val127-Ala340 of the  $\alpha 1$  chain was amplified from full length cDNAs by the polymerase chain reaction (PCR) (PCR CORE Kit; Boehringer Mannheim, GmbH Germany), using rat specific primers (5'-CAGGATCCGTCAGTCCTACATTTCAA-3' [forward][SEQ ID NO: 1]; 5'-TCCTCGAGCGCTTCCAAAGCGAATAT-3' [reverse]{SEQ ID NO: 2].

The resulting PCR amplified products were purified over a PCR select II column (5 prime-3 prime), digested with Bam H1 and Xho 1 restriction enzymes, re-purified over a PCR select II column, and ligated in pGEX4t (Pharmacia), previously digested with Bam H1 and Xho1, dephosphorylated with calf intestinal alkaline phosphatase (New England Biolabs), and gel purified. Ligation products were transformed into competent DH5A E.Coli cells (Gibco BRL) and the resulting amplicillin resistant colonies were screened for the expression of the ~45 kDa glutathione S-transferase-I domain fusion protein. The I-domain was expressed as a GST fusion protein with a thrombin cleavage site at the junction of the sequences.

Cells in PBS (1 part of wet cell weight to 4 parts of buffer) were lysed in a Gaulin press and clarified of particulates by centrifugation (14,000 x g, 30 min). 650 ml of lysate from 180 g of cell paste was loaded onto a 25 ml glutathione Sepharose 4B column (Pharmacia). The column was washed with 100 ml of PBS and the rat alpha1 integrin I domain-GST fusion protein eluted from the column with 50 mM Tris HCl pH 8.0, 5 mM glutathione (reduced). Five ml fractions were collected and analyzed for total protein by absorbance at 280 nm and for purity by SDS-PAGE. Peak fractions were pooled, aliquoted, and stored at –70 degrees C. A total of 375 mg of the fusion protein (15 mg/ml) at >90% purity was recovered.

For preparation of the purified I-domain, 6 ml of the fusion protein was dialyzed overnight against one liter of 50 mM Tris pH 7.5. The sample was treated with 100 µg of thrombin (a gift of Dr. John Fenton, New York State Department of Health, Albany, NY) for 150 min at room temperature. DTT was added to 2 mM and the sample was loaded onto a 7 ml glutathione Sepharose® 4B column. The flow through from the column was collected as 1.5 ml fractions and the column was further washed with 50 mM Tris HCl pH 7.5, 2 mM DTT buffer. The flow through and wash fractions were analyzed for

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absorbance at 280 nm. Peak fractions were pooled and loaded onto a 2.4 ml Q Sepharose® FF column (Pharmacia).

The Q-Sepharose column was washed with 2 ml of 50 mM Tris HCl pH 7.5, 2 mM DTT; 2 ml of 50 mM Tris HCl pH 7.5, 10 mM 2-mercaptoethanol; twice with 2ml of 50 mM Tris HCl pH 7.5, 10 mM 2-mercaptoethanol, 25 mM NaCl; and the alpha 1 integrin I domain eluted with 50 mM Tris HCl pH 7.5, 10 mM 2-mercaptoethanol, 75 mM NaCl. Peak fractions were pooled, filtered through a 0.2 μm filter, and stored at 4 degrees C. The final product was >99% pure by SDS-PAGE, eluted as a single peak by size exclusion chromatography on a Superose® 6 column (Pharmacia & Upjohn) consistent with its predicted mass, and by electrospray ionization-mass spectrometry (ESI-MS, Micromass, Quattro-II, Manchester, UK) contained a single ion with mass of 24,868 Da, which agreed with the predicted mass of 24871.2 Da for the rat α1 I-domain sequence plus the GS linker resulting from cleavage at the engineered thrombin cleavage site. From 72 mg of the fusion protein, 24 mg of the purified I- domain was recovered (based on a theoretical extinction coefficient of 0.5 at 280 nm for 1 mg/ml solution of the I-domain).

In preliminary studies, we found that the rat  $\alpha 1$  integrin I-domain in this form failed to crystallize under any test condition and, as had been observed for other I domains (R.Liddington, personal communication), that sequences at the N-terminus of the I domain construct were problematic. A simple proteolytic method was developed to convert the purified rat I-domain into a form that could be crystallized.

Briefly, 240 µl of the purified alpha 1 integrin I domain (16 mg/ml) was diluted with 360 µl of 50 mM Tris HCl pH 7.5 and loaded onto a 1.2 ml V8 protease column (Pierce) that had been equilibrated in 50 mM Tris HCl pH 7.5. The I domain solution was left in contact with the resin for 35 min at room temperature and then recovered by washing the column with 50 mM Tris HCl pH 7.5. The I domain was then dialyzed overnight against 10 mM Tris pH 7.5, 10 mM 2-mercaptoethanol and concentrated to 11 mg/ml in a centricon-10 ultrafiltration unit (Amicon). ESI-MS analysis of V8 protease digested product revealed that the product had been converted into a des 1-18 form, starting at Cys143 in the fusion protein construct.

#### B. Crystallization

Buffer chemicals were purchased from Fisher (Boston, MA). Crystallization condition screenings were done with the Crystal Screen I kit from Hampton Research

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(Riverside, CA). Crystals were grown by the vapor diffusion method of Jancarik & Kim (1991) J. Appl. Crystallogr. 24, 409-411.

In order to find conditions of crystallization, an incomplete factorial screen was set up. In a typical experiment, protein solution was mixed with an equal volume of reservoir solution and a drop of the mixture was suspended under a glass cover slip over the reservoir solution. Crystals were grown out of 25% w/v Polyethylene Glycol (PEG) 8000, 0.1 M sodium cacodylate pH 6.5, 0.2 M sodium acetate reservoir solution. The crystals are shaped as plates, are easy to reproduce and can reach maximum dimensions of almost 0.5 mm on one side. Variation of pH between 6 and 7 did not affect crystal quality.

Those of skill in the art will appreciate that the aforesaid crystallization conditions can be varied. By varying the crystallization conditions, other crystal forms of  $\alpha1\beta1$  integrin I-domain may be obtained. Such variations may be used alone or in combination, and include: varying final protein concentrations between 5 mg/ml and 35 mg/ml; varying the s $\alpha1\beta1$  integrin I-domain to precipitant ratio; varying PEG concentrations between 15% and 35% w/v; varying the molecular weight of polyethylene glycol from 400 to 8000; varying pH ranges between 5.0 and 9.5; varying sodium cacodylate concentrations between 5 and 395 mM; varying sodium acetate concentrations between 5 and 495 mM; varying the concentration or type of detergent; varying the temperature between -5 degrees C and 30 degrees C; and crystallizing  $\alpha1\beta1$  integrin I-domain by batch, liquid bridge, or dialysis method using the above conditions or variations thereof. See McPherson, A.(1982). Preparation and Analysis of Protein Crystals. (Glick, ed.) pp. 82-159, John Wiley & Co., N.Y., specifically incorporated by reference herein.

# C. Data collection and processing

Crystals were equilibrated gradually in a cryoprotectant solution of 20% glycerol, 25% w/v PEG 8000, 0.1 M sodium cacodylate pH 6.5, 0.2 M sodium acetate, and were mounted on a loop and immediately frozen in a -150 C liquid nitrogen gas stream. The technique of freezing the crystals essentially immortalizes them and produced a much higher quality data set.

A native X-ray data set up to 3.0 Å resolution was collected from one crystal by using an R-AXIS II image plate detector system (Molecular Structure Corporation, Woodlands, TX). A second data set to 2.2 Å resolution was collected later by using a

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larger crystal. The data were integrated and reduced using the HKL program package (Otwinowski et al (1993) in Data collection and Processing pp 80-86, SERC Daresbury Laboratory, Warrington, UK ). The data collection required about 4 days. Data processing suggested an orthorhombic unit cell with approximate cell dimensions a=34.77 Å , b=85.92 c=132.56 and alpha=beta=gamma=90. The space group was identified as  $P2_12_12_1$ . The 2.2 Å data set was 91.3% complete and had an R-merge of 5.6%. Calculation of the Matthews volume gives  $V_M = 4.22$  assuming a molecular weight of 23,000 daltons which suggested that there are 2 molecules in the asymmetric unit.

#### D. Molecular replacement

All subsequent molecular replacement computing was done with the program Amore (Navaja et al (1994) Acta Crystallogr. A 50, 157-163) from the CCP4 program package (The SERC (UK) Collaborative Computing Project No 4, Daresbury Laboratory, UK 1979). Molecular graphics manipulations were done with QUANTA (Molecular Simulations, Inc.) and "O" software (Jones et al 1991 Acta Crystallogr. A 47, 110-119). The coordinates of the crystal structure of the human α2 I-domain (Emsley et al. (1997) J. Biol.Chem. 272, 28512-28517) was used as a probe for rotation and translation searches using the 3 Å data set.

We used all the coordinates of all atoms, including side chains. The rotation function gave a solution with the highest correlation coefficient (cc) of 9.7. This solution was used for a first translation function which yielded a cc of 24.6 and an R-factor of 48.7%. Using rigid body refinement, these values refined to cc=40.3, R-factor=48.7%. Using this first solution, we took the peaks of the first rotation search and used these for searching the second molecule, keeping our first solution fixed. The translation search yielded a maximum peak with cc=37.3 and an R-factor of 44.8%. Rigid body refinement on these two solutions resulted in cc=56.3 and R-factor=43.3%.

The next highest solution gave: cc=36.6 R-fac=49.9%. By generating symmetry related molecules and displaying them with computer graphics it was found that they packed satisfactorily in the unit. The rotation matrix between the two molecules of the asymmetric unit was determined and one molecule was used for the initial stages of model building.

# E. Model building and crystallographic refinement

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All subsequent refinement computing was done with the XPLOR program (Brunger et al (1987) Science 235, 458-460). 10% of the data were used for the calculation of R-free. To reduce model bias, partial models were used for map calculation and refinement. The initial partial model, containing a polyalanine chain of the secondary structure elements only, from the a2 I-domain structure, was subjected to conventional positional refinement and grouped B-factor refinement with strict non -crystallographic symmetry constraints.

The R and R-free factors dropped to 32.3% and 39.4% respectively. 3Fo -2Fc maps were used for cycles of model building and refinement. The resolution range used was from 8 to 3 Å. Typically, cycles consisted of model building, positional refinement and B-factor refinement. When the R and R-free reached 26% and 36% respectively, the 3 Å data set did not allow further improvement of the model. The 2.2 Å data set was collected at this point and was used for all subsequent model building and refinement. The R and R-free factors after the initial rigid body refinement at 2.2 Å were 41.3% and 42.2% respectively.

This larger data set allowed use of simulated annealing refinement and torsion angle dynamics refinement. As the phases improved, more atoms were added into the model. Initially, grouped B-factors were assigned for each residue (one for main chain and the one for side chain atoms). Later, non-crystallographic symmetry constraints were removed and individual atomic B-factors where refined for each residue. In addition bulk solvent correction was applied to the data set. Residues and side chains would be incorporated in the model if they were sufficiently well defined in 3Fo-2Fc electron density maps. Only manual structure modifications that resulted in lower R-free after refinement were accepted.

When R and R-free reached 29% and 34.8% respectively, water molecules were added by using the X-solvate utility of QUANTA. Finally, maximum likelihood refinement was used (Adams et al (1997) Pro.Nat.Acad.Sci USA 94, pp. 5018-5023) and resulted in the final structure with R and R-free of 23.5% and 30.2% respectively for data between 100 and 2.2 Å resolution. Table I summarizes information regarding crystallographic data and refinement. Table II lists the atomic coordinates of the I-domain of the  $\alpha$ 1 chain of the rat  $\alpha$ 1 $\beta$ 1 integrin. The coordinates of the crystal structure of the I-

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by the small molecule.

domain may be used in the structure-based design of small molecule inhibitors of  $\alpha 1\beta 1$ , computational drug design and iterative structure optimization.

#### a. Computational drug design

Small molecule inhibitors can be designed using computational approaches. These approaches are also known as de novo drug design. In brief, the crystal structure coordinates of the  $\alpha 1\beta 1$  integrin or fragment(s) thereof are the input for a computer program, such as DOCK. Programs such as DOCK output a list of small molecule structures that are expected to bind to  $\alpha 1\beta 1$  or the fragment(s). These molecules can then be screened by biochemical assays for a1\beta1 binding. Typically, biochemical assays that screen molecules for their ability to bind to  $\alpha 1 \beta 1$  or a fragment thereof are competitiontype assays. In such assays, the molecule is added to the assay solution and the degree of inhibition is measured using conventional methodology. An example of such an assay is the following: 96 well plates can be coated with collagen IV or collagen I and blocked with 3% Bovine Serum Albumin solution. Solution of a1 Idomain together with the small molecule under testing are incubated on the coated plates at room temperature for 1 hour and washed in triton buffer. Bound a1 I-domain is detected with a biotinylated anti-I-domain antibody. Plates are read at OD<sub>405</sub> on a microplate reader. The amount of bound I-domain is compared with a control experiment with no small molecule present. If it is lower than that of the control experiment that suggests inhibition

#### b. Iterative cycles of structure optimization

The crystal structures of complexes formed between  $\alpha 1\beta 1$  or a fragment and small molecule inhibitors may be solved. In brief, small molecule inhibitors are typically found using the crystal structure coordinates of a s $\alpha 1\beta 1$  integrin or fragment either by the computational approaches mentioned above or by the screening of small molecule libraries. The small molecule inhibitor is then co-crystallized with  $\alpha 1\beta 1$  or a fragment and the crystal structure of the complex is solved by molecular replacement. Molecular replacement requires the coordinates of a s $\alpha 1\beta 1$  or fragment for the calculation of phases. The information collected from these experiments can be used to optimize the structure of small molecule inhibitors by clarifying how small molecules interact with the protein target. This suggests ways of modifying the small molecule to improve its

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physicochemical properties, such as affinity, specificity, and kinetics with regard to the  $\alpha 1\beta 1$  target.

In addition to being necessary for computational drug design and structure optimization, the crystal coordinates described herein are useful for analyzing the  $\alpha 1\beta 1$  binding site. Through such analysis, it was determined that a particularly attractive region for drug targeting is in the vicinity of residues Asp154, Ser156, Asn157, Ser158, Leu222, Gln223, Thr224, Asp257, Glu259, His261, His288, Tyr289, Gly292, Leu294 and Lys298. The above observations and hypotheses suggest that this region may contribute significantly to the binding energy of  $\alpha 1\beta 1/ECM$  interactions, and therefore, is an attractive target for inhibitor design. Site mutations studies can be used in conjunction with the above-described processes to further define the binding site.

It will be apparent to those skilled in the art that various modifications and variations can be made in the methods and compositions of the present invention without departing from the spirit or scope of the invention. Thus, it is intended that the present invention cover the modifications and variations of this invention provided that they come within the scope of the appended claims and their equivalents.

TABLE I: Crystallographic data statistics:

 $P2_12_12_1$ Symmetry: a = 34.77, b = 85.92, c = 132.5620 Unit cell (Å) 1 No.of crystals: Resolution (Å) 2.2 Reflections(unique): 19,238 5.6%  $R_{\text{merge}}$ 91.3% 25 Completeness: Completeness(2.2-2.28 Å) 77.6%

TABLE II: Crystallographic coordinates of the alpha1 I-domain crystal structure in PDB(XPLOR) format. Segment names A, B, W correspond to molecule A, molecule B and water respectively.

CRYST	34.	770	85.	920 132	.560 90.00	90.00	90.00	P212121	
ATOM	1	CB	ALA	145	35.261	87.828	-14.480	1.00 46.82	A
ATOM	2	С	ALA	145	33.051	87.078	-15.373	1.00 48.98	A
АТОМ	3	0	ALA	145	32.414	87.150	-14.310	1.00 49.22	A
ATOM	4	HT1	ALA	145	33.390	89.717	-14.876	1.00 0.00	A
ATOM	5	HT2	ALA	145	33.206	89.509	-16.551	1.00 0.00	A
ATOM	6	N	ALA	145	33.860	89.407	-15.751	1.00 47.03	A
ATOM	7	HT3	ALA	145	34.705	89.992	-15.916	1.00 0.00	A
ATOM	8	CA	ALA	145	34.266	87.977	-15.619	1.00 46.67	A
	ATOM ATOM ATOM ATOM ATOM ATOM ATOM	ATOM 1 ATOM 2 ATOM 3 ATOM 4 ATOM 5 ATOM 6 ATOM 7	ATOM 1 CB ATOM 2 C ATOM 3 O ATOM 4 HT1 ATOM 5 HT2 ATOM 6 N ATOM 7 HT3	ATOM 1 CB ALA ATOM 2 C ALA ATOM 3 O ALA ATOM 4 HT1 ALA ATOM 5 HT2 ALA ATOM 6 N ALA ATOM 7 HT3 ALA	ATOM 1 CB ALA 145 ATOM 2 C ALA 145 ATOM 3 O ALA 145 ATOM 4 HT1 ALA 145 ATOM 5 HT2 ALA 145 ATOM 6 N ALA 145 ATOM 7 HT3 ALA 145	ATOM 1 CB ALA 145 35.261 ATOM 2 C ALA 145 33.051 ATOM 3 O ALA 145 32.414 ATOM 4 HT1 ALA 145 33.390 ATOM 5 HT2 ALA 145 33.206 ATOM 6 N ALA 145 33.860 ATOM 7 HT3 ALA 145 34.705	ATOM 1 CB ALA 145 35.261 87.828 ATOM 2 C ALA 145 33.051 87.078 ATOM 3 O ALA 145 32.414 87.150 ATOM 4 HT1 ALA 145 33.390 89.717 ATOM 5 HT2 ALA 145 33.206 89.509 ATOM 6 N ALA 145 33.860 89.407 ATOM 7 HT3 ALA 145 34.705 89.992	ATOM 1 CB ALA 145 35.261 87.828 -14.480 ATOM 2 C ALA 145 33.051 87.078 -15.373 ATOM 3 O ALA 145 32.414 87.150 -14.310 ATOM 4 HT1 ALA 145 33.390 89.717 -14.876 ATOM 5 HT2 ALA 145 33.206 89.509 -16.551 ATOM 6 N ALA 145 33.860 89.407 -15.751 ATOM 7 HT3 ALA 145 34.705 89.992 -15.916	ATOM 1 CB ALA 145 35.261 87.828 -14.480 1.00 46.82 ATOM 2 C ALA 145 33.051 87.078 -15.373 1.00 48.98 ATOM 3 O ALA 145 32.414 87.150 -14.310 1.00 49.22 ATOM 4 HT1 ALA 145 33.390 89.717 -14.876 1.00 0.00 ATOM 5 HT2 ALA 145 33.206 89.509 -16.551 1.00 0.00 ATOM 6 N ALA 145 33.860 89.407 -15.751 1.00 47.03 ATOM 7 HT3 ALA 145 34.705 89.992 -15.916 1.00 0.00

	MOTA	9	N	ALA	146	32.737		-16.358	1.00 42.12	A
	ATOM	10	H	ALA	146	33.287		-17.170	1.00 0.00	A
	ATOM	11	CA	ALA	146	31.603		-16.264	1.00 40.10	A
_	ATOM	12	СВ	ALA	146	31.657 31.621		-17.389 -14.919	1.00 35.92 1.00 40.80	A A
5	ATOM	13 14	C 0	ALA ALA	146 146	32.511		-14.647	1.00 42.91	A
	ATOM ATOM	15	И	LEU	147	30.629		-14.082	1.00 37.99	A
	ATOM	16	H	LEU	147	29.931		-14.359	1.00 0.00	A
	ATOM	17	CA	LEU	147	30.562	84.284	-12.759	1.00 37.93	A
10	ATOM	18	CB	LEU	147	31.411		-11.803	1.00 38.26	A
	MOTA	19	CG	LEU	147	31.994		-10.623	1.00 39.33	A
	ATOM	20		LEU	147	33.183		-11.078	1.00 33.15 1.00 38.31	A A
	ATOM	21		LEU	147	32.389 29.156	85.347	-9.567 -12.181	1.00 36.60	A
15	ATOM	22 23	C 0	LEU LEU	$147 \\ 147$	28.417		-12.132	1.00 37.06	A
13	ATOM ATOM	24	N	ASP	148	28.780		-11.751	1.00 36.31	A
	ATOM	25	Н	ASP	148	29.384		-11.844	1.00 0.00	A
	ATOM	26	CA	ASP	148	27.468		-11.140	1.00 33.40	A
	MOTA	27	CB	ASP	148	26.836		-11.589	1.00 35.41	A
20	MOTA	28	CG	ASP	148	26.085		-12.925	1.00 33.40 1.00 32.84	A A
	MOTA	29		ASP	148	25.783 25.795		-13.531 -13.376	1.00 32.64	A
	ATOM ATOM	30 31	C C	ASP ASP	148 148	27.695	82.829	-9.622	1.00 28.37	A
	ATOM	32	0	ASP	148	28.475	82.050	-9.070	1.00 26.95	A
25	ATOM	33	N	ILE	149	27.027	83.767	-8.961	1.00 25.21	A
	MOTA	34	H	ILE	149	26.411	84.349	-9.453	1.00 0.00	A
	ATOM	35	CA	ILE	149	27.179	83.957	-7.529	1.00 24.78	A
	ATOM	36	CB	ILE	149	27.883	85.308 85.509	-7.229 -5.718	1.00 25.55 1.00 19.80	A A
20	ATOM	37		ILE	149 149	28.047 29.233	85.363	-7.947	1.00 13.80	A
30	ATOM ATOM	38 39		ILE ILE	149	29.730	86.775	-8.168	1.00 25.74	A
	ATOM	40	C	ILE	149	25.853	83.957	-6.786	1.00 27.12	A
	ATOM	41	0	ILE	149	24.957	84.737	-7.097	1.00 27.87	A
	ATOM	42	N	VAL	150	25.748	83.101	-5.780	1.00 29.44	A
35	ATOM	43	H	VAL	150	26.498	82.509	-5.564	1.00 0.00 1.00 31.56	A A
	ATOM	44	CA	LAV	150 150	24.525 23.914	83.031 81.612	-4.990 -5.015	1.00 31.56	A
	ATOM ATOM	45 46	CB CG1	VAL VAL	150	22.921	81.433	-3.871	1.00 36.22	A
	ATOM	47		VAL	150	23.218	81.387	-6.339	1.00 35.65	A
40	ATOM	48	C	VAL	150	24.751	83.443	-3.543	1.00 29.32	A
	MOTA	49	0	VAL	150	25.643	82.939	-2.849	1.00 27.25	A
	MOTA	50	N	ILE	151	23.936	84.383	-3.096	1.00 29.18 1.00 0.00	A A
	ATOM	51	H	ILE	151 151	23.269 24.016	84.772 84.847	-3.699 -1.724	1.00 28.46	A
45	ATOM ATOM	52 53	CA CB	ILE	151	23.614	86.340	-1.625	1.00 27.62	A
43	MOTA	54	CG2		151	23.843	86.860	-0.209	1.00 24.70	A
	MOTA	55		ILE	151	24.457	87.167	-2.607	1.00 27.55	A
	MOTA	56		ILE	151	23.788	87.443	-3.933	1.00 28.07	A
50	MOTA	57	C		151	23.067	83.964 83.721	-0.908 -1.307	1.00 26.00 1.00 25.72	A A
50	ATOM	58 59	O N	ILE VAL	151 152	21.923 23.575	83.445		1.00 23.72	A
	ATOM ATOM	60	H	VAL	152	24.506	83.650		1.00 0.00	A
	ATOM	61	CA	VAL	152	22.813	82.581	1.099	1.00 23.05	A
	ATOM	62	CB	VAL	152	23.585	81.247		1.00 26.59	A
55	MOTA	63		. VAL	152	22.665	80.246		1.00 25.59 1.00 21.54	A A
	ATOM	64		VAL	152	24.102 22.689	80.628 83.412		1.00 21.54	A
	ATOM	65 66	C O	$\overline{ ext{VAL}}$	152 152	23.554	83.369		1.00 20.44	A
	ATOM ATOM	67	N	LEU	153	21.613	84.180		1.00 20.46	A
60	ATOM	68	H	LEU	153	20.950	84.144		1.00 0.00	A
	ATOM	69	CA	LEU	153	21.384	85.071		1.00 19.62	A
	MOTA	70	CB	LEU	153	20.780	86.370		1.00 27.82	A
	ATOM	71	CG	LEU	153	20.357	87.482		1.00 29.39 1.00 32.60	A A
65	ATOM	72		LEU	153	21.555 19.683	88.057 88.565		1.00 32.00	A
65	ATOM ATOM	73 74	CD2	LEU LEU	153 153	20.518	84.490		1.00 34.32	A
	ATOM	75	Ö	LEU	153	19.360	84.122		1.00 20.87	A
	ATOM	76	N	ASP	154	21.101	84.430	5.846	1.00 20.52	A
	MOTA	77	H	ASP	154	22.026	84.747		1.00 0.00	A
70	MOTA	78	CA	ASP	154	20.439	83.917		1.00 20.46	A A
	ATOM	79	CB	ASP	154	21.506	83.624 83.418		1.00 22.44 1.00 20.33	A A
	MOTA	80 81	CG OD1	ASP L ASP	154 154	20.946 19.773	83.418		1.00 25.28	A
	MOTA	OΤ	נעט	LADE	174	27.775	JJ. U.	5.047		

	ATOM	82	OD2	ASP	154	21.709	83.658	10.408	1.00 17.38	A
	ATOM	83		ASP	154	19.463	85.012	7.445	1.00 24.81	A
	ATOM	84		ASP	154	19.850	86.170	7.680	1.00 19.94	A
	ATOM	85		GLY	155	18.186	84.645	7.491	1.00 22.66	A
5	ATOM	86	H	GLY	155	17.945	83.724	7.270	1.00 0.00	A
	MOTA	87	CA	GLY	155	17.154	85.583	7.865	1.00 25.80	A
	ATOM	88	С	GLY	155	16.573	85.333	9.242	1.00 27.90	A
	MOTA	89	0	GLY	155	15.411	85.623	9.465	1.00 30.07	A
	MOTA	90	N	SER	156	17.363	84.783	10.158	1.00 29.73	A
10	ATOM	91	H	SER	156	18.280	84.539	9.917	1.00 0.00	A
	ATOM	92	CA	SER	156	16.887	84.533	11.519	1.00 33.03 1.00 33.06	A A
	ATOM	93	CB	SER	156	17.956	83.778	12.327	1.00 33.00	A
	ATOM	94	OG	SER	156	18.696	84.658 84.158	13.163 13.652	1.00 34.40	A
1.5	ATOM	95	HG	SER	156	19.354 16.589	85.896	13.032 $12.162$	1.00 28.30	A
15	ATOM	96	C	SER SER	156 156	16.928	86.935	11.595	1.00 32.92	A
	ATOM ATOM	97 98	N	ASN	157	15.958	85.892	13.335	1.00 27.00	A
	ATOM	99	H	ASN	157	15.732	85.033	13.746	1.00 0.00	A
	ATOM	100	CA	ASN	157	15.591	87.140	14.032	1.00 22.66	A
20	ATOM	101	CB	ASN	157	14.545	86.871	15.127	1.00 24.65	A
20	ATOM	102	CG	ASN	157	13.322	86.095	14.644	1.00 26.95	A
	ATOM	103	OD1		157	12.722	85.354	15.422	1.00 22.76	A
	ATOM	104	ND2	ASN	157	12.941	86.269	13.380	1.00 23.43	A
	ATOM	105	HD21	ASN	157	13.442	86.879	12.800	1.00 0.00	A
25	MOTA	106	HD22	ASN	157	12.156	85.772	13.074	1.00 0.00	A
	MOTA	107	C	ASN	157	16.724	87.922	14.717	1.00 20.73	A
	MOTA	108	0	ASN	157	16.488	89.024	15.179	1.00 19.35	A
	ATOM	109	N	SER	158	17.936	87.382	14.804 14.395	1.00 20.15 1.00 0.00	A A
20	ATOM	110	H	SER	158	18.117 19.005	86.511 88.099	15.519	1.00 17.25	A
30	ATOM	111	CA	SER SER	158 158	20.003	87.095	16.115	1.00 17.23	A
	ATOM	112 113	CB OG	SER	158	20.309	86.048	15.204	1.00 21.49	A
	ATOM ATOM	114	HG	SER	158	20.692	86.418	14.407	1.00 0.00	A
	ATOM	115	C	SER	158	19.764	89.191	14.750	1.00 19.11	A
35	ATOM	116	ŏ	SER	158	20.168	90.196	15.331	1.00 15.49	A
	MOTA	117	N	ILE	159	19.985	88.994	13.462	1.00 19.24	A
	ATOM	118	H	ILE	159	19.683	88.164	13.037	1.00 0.00	A
	ATOM	119	CA	ILE	159	20.674	90.002	12.670	1.00 24.70	A
	MOTA	120	CB	ILE	159	20.702	89.596	11.193	1.00 25.84	A
40	MOTA	121	CG2		159	21.185	90.750	10.347	1.00 23.12	A A
	MOTA	122	CG1		159	21.602	88.366	11.029 10.092	1.00 30.68 1.00 36.48	A
	MOTA	123		ILE	159	21.058 19.755	87.313 91.188	12.863	1.00 30.40	A
	MOTA	124 125	C	ILE ILE	159 159	18.733	91.293	12.201	1.00 27.59	A
45	MOTA MOTA	126	N	TYR	160	20.099	92.098	13.764	1.00 32.64	A
45	MOTA	127	H	TYR	160	20.953	92.057	14.240	1.00 0.00	A
	ATOM	128	CA	TYR	160	19.142	93.153	13.995	1.00 36.31	A
	ATOM	129	СВ	TYR	160	19.262	93.759	15.384	1.00 29.60	A
	MOTA	130	CG	TYR	160	18.250	94.871	15.541	1.00 25.36	A
50	MOTA	131	CD1	TYR	160	16.953	94.731	15.034	1.00 30.44	A
	MOTA	132	CE1		160	16.027	95.768	15.113	1.00 28.80	A
	$\mathbf{MOTA}$	133	CD2		160	18.597	96.077	16.131	1.00 22.43 1.00 29.79	A A
	ATOM	134			160	17.686	97.118 96.958	16.218 15.706	1.00 29.79	A
	MOTA	135		TYR	160	16.406 15.514	97.989	15.801	1.00 35.06	A
55	MOTA	136		TYR	160 160	14.682	97.730	15.399	1.00 0.00	A
	MOTA	137 138		TYR TYR	160	19.015	94.279	13.018	1.00 38.57	A
	ATOM ATOM	139		TYR	160	18.019	94.342	12.297	1.00 45.05	A
	ATOM	140		PRO	161	19.992	95.194	12.969	1.00 34.46	A
60	ATOM	141		PRO	161	21.298	95.354	13.624	1.00 23.12	A
-	ATOM	142		PRO	161	19.727	96.237	11.978	1.00 32.11	A
	ATOM	143	CB	PRO	161	20.946	97.155	12.068	1.00 30.05	A
	MOTA	144	CG	PRO	161	21.657	96.769	13.287	1.00 34.00	A
	MOTA	145	C	PRO	161	19.578	95.579	10.605	1.00 30.24	A
65	ATOM	146		PRO	161	20.555	95.434	9.878	1.00 29.38	A
	ATOM	147		TRP	162	18.365	95.167	10.254	1.00 28.87	A A
	MOTA	148		TRP	162	17.603	95.296	10.855	1.00 0.00 1.00 29.54	A A
	ATOM	149		TRP	162	18.180	94.525 94.114	8.970 8.744	1.00 29.34	A
70	ATOM	150		TRP	162 162	16.725 16.577	93.324	7.456	1.00 27.54	A
70	ATOM	151		TRP TRP	162	17.115	92.017	7.176	1.00 27.34	A
	MOTA MOTA	152 153			162	16.795	91.710	5.837	1.00 27.60	A
	ATOM	154		TRP	162	17.831	91.081	7.935	1.00 22.75	A

	MOTA	155 CD1 TRE		15.976	93.740	6.304	1.00 27.18	A
	ATOM ATOM	156 NE1 TRE 157 HE1 TRE		16.103 15.756	92.779 92.847	5.324 4.416	1.00 31.45 1.00 0.00	A A
	ATOM	158 CZ2 TRI		17.169	90.503	5.230	1.00 25.17	A
5	MOTA	159 CZ3 TRE		18.201	89.879	7.343	1.00 21.51	A
	MOTA	160 CH2 TRE		17.872	89.601	5.998	1.00 27.23	A
	ATOM	161 C TRI 162 O TRI		18.644 19.318	95.419 94.945	7.825 6.914	1.00 32.23 1.00 29.79	A A
	ATOM ATOM	162 O TRI 163 N GLU		18.314	96.708	7.859	1.00 34.04	A
10	ATOM	164 H GLU		17.794	97.072	8.607	1.00 0.00	A
	ATOM	165 CA GLU		18.744	97.572	6.757	1.00 36.74	A
	MOTA	166 CB GLU		18.235	99.011	6.936 8.355	1.00 33.42 1.00 41.87	A
	ATOM ATOM	167 CG GLU 168 CD GLU		17.941 18.085	99.437 100.938	8.529	1.00 41.87	A A
15	ATOM	169 OE1 GLU		19.238	101.426	8.588	1.00 44.11	A
	ATOM	170 OE2 GLU		17.047	101.629	8.597	1.00 39.73	A
	MOTA	171 C GLU		20.267	97.578	6.566	1.00 35.78	A
	ATOM	172 O GLU		20.769 20.987	98.002 97.083	5.519 7.574	1.00 29.20 1.00 35.57	A A
20	ATOM ATOM	173 N SEI 174 H SEI		20.516	96.748	8.364	1.00 0.00	A
20	ATOM	175 CA SEI		22.443	97.024	7.547	1.00 31.38	A
	MOTA	176 CB SEE		22.990	96.956	8.968	1.00 30.80	A
	ATOM	177 OG SEI		22.876	98.211	9.605	1.00 37.22	A
25	MOTA ATOM	178 HG SEI 179 C SEI		23.225 22.964	98.151 95.837	10.498 6.751	1.00 0.00 1.00 32.24	A A
23	ATOM	180 O SEI		24.084	95.870	6.231	1.00 37.08	A
	ATOM	181 N VA		22.171	94.775	6.688	1.00 31.62	A
	MOTA	182 H VAI		21.316	94.783	7.165	1.00 0.00	A
30	ATOM ATOM	183 CA VAI 184 CB VAI		22.553 21.623	93.602 92.401	5.916 6.164	1.00 31.01 1.00 35.77	A A
30	ATOM	185 CG1 VAI		22.339	91.110	5.787	1.00 39.39	A
	ATOM	186 CG2 VA	165	21.177	92.366	7.607	1.00 40.80	A
	ATOM	187 C VAI		22.328	94.049	4.493	1.00 32.48	A
35	MOTA	188 O VAI 189 N ILI		23.156 21.187	93.824 94.701	3.609 4.297	1.00 35.34 1.00 33.35	A A
33	ATOM ATOM	189 N ILI 190 H ILI		20.586	94.837	5.058	1.00 0.00	A
	ATOM	191 CA IL		20.789	95.225	2.997	1.00 32.78	A
	ATOM	192 CB IL		19.382	95.862	3.078	1.00 31.47	A
40	ATOM	193 CG2 ILI		19.056 18.346	96.575 94.785	1.783 3.419	1.00 32.21 1.00 30.98	A A
40	ATOM ATOM	194 CG1 ILI 195 CD1 ILI		16.917	95.142	3.048	1.00 25.05	A
	ATOM	196 C IL		21.800	96.267	2.504	1.00 30.96	A
	MOTA	197 O IL		22.159	96.293	1.326	1.00 31.98	A
45	ATOM	198 N AL		22.260 21.947	97.120 97.057	3.410 4.337	1.00 31.52 1.00 0.00	A A
43	ATOM ATOM	199 H AL. 200 CA AL.		23.228	98.153	3.047	1.00 33.64	A
	ATOM	201 CB AL		23.540	99.023	4.253	1.00 29.88	A
	MOTA	202 C AL		24.502	97.482	2.539	1.00 35.05	A
50	ATOM	203 O AL		25.176 24.821	97.982 96.342	3.141	1.00 30.30 1.00 31.11	A A
30	ATOM ATOM	204 N PH: 205 H PH:		24.245	96.013	3.864	1.00 0.00	A
	ATOM	206 CA PH		25.987	95.572	2.771	1.00 28.96	A
	MOTA	207 CB PH		26.214	94.504	3.835	1.00 32.92	A
55	ATOM ATOM	208 CG PH 209 CD1 PH		27.007 26.378	93.329 92.118	3.371 3.111	1.00 29.30 1.00 31.94	A A
33	ATOM	210 CD2 PH		28.386	93.405	3.266	1.00 26.68	A
	ATOM	211 CE1 PH		27.104		2.760	1.00 28.37	A
	MOTA	212 CE2 PH		29.128	92.282	2.913	1.00 31.48	A
60	ATOM	213 CZ PH		28.481 25.736	91.071 94.955	2.660 1.395	1.00 33.94 1.00 30.36	A A
60	MOTA MOTA	214 C PH 215 O PH		26.549		0.482	1.00 35.57	A
	ATOM	216 N LE		24.602	94.279	1.241	1.00 29.42	A
	ATOM	217 H LE		23.985		1.997	1.00 0.00	A
65	ATOM	218 CA LE		24.262	93.666	-0.037 -0.008	1.00 32.92 1.00 30.46	A A
65	MOTA MOTA	219 CB LE 220 CG LE		22.835 22.485		0.773	1.00 30.46	A A
	ATOM	221 CD1 LE		21.107		0.309	1.00 23.84	A
	ATOM	222 CD2 LE		23.504	90.738	0.549	1.00 22.89	A
	MOTA	223 C LE		24.371		-1.148	1.00 36.13	A
70	MOTA	224 O LE		24.992 23.760		-2.181 $-0.920$	1.00 37.86 1.00 39.95	A A
	MOTA MOTA	225 N AS 226 H AS		23.279		-0.920	1.00 39.93	A
	ATOM	227 CA AS		23.779		-1.882	1.00 35.60	A

	ATOM	228 C	B ASN	170	23.040	98.179	-1.275	1.00 40.87	A
	ATOM	229 C	G ASN	170	23.122	99.427	-2.140	1.00 45.43	A
	ATOM	230 O	D1 ASN	170	24.008 1	100.268	-1.958	1.00 38.53	A
	MOTA	231 N	D2 ASN	170	22.191	99.558	-3.083	1.00 44.25	A
5	MOTA	232 HD		170	21.503	98.868	-3.188	1.00 0.00	A
	ATOM	233 HD		170	22.229 1		-3.648	1.00 0.00	A
	MOTA	234 C	ASN	170	25.221	97.354	-2.203	1.00 37.08	A
	ATOM	235 0		170	25.590	97.546	-3.360	1.00 36.45 1.00 41.63	A A
10	MOTA	236 N		171	26.022	97.444 97.256	-1.149 $-0.267$	1.00 41.03	A
10	ATOM	237 H		171 171	25.640 27.430	97.236	-1.219	1.00 45.96	A
	MOTA	238 C. 239 C.		171	27.984	97.921	0.205	1.00 49.80	A
	ATOM ATOM	240 C		171	28.976	99.051	0.360	1.00 58.06	A
	ATOM		D1 ASP	171		100.218	0.111	1.00 61.54	А
15	ATOM		D2 ASP	171	30.131	98.771	0.738	1.00 60.67	A
10	MOTA	243 C		171	28.286	96.815	-2.018	1.00 47.51	A
	ATOM	244 0		171	29.263	97.214	-2.656	1.00 45.54	A
	MOTA	245 N	LEU	172	27.923	95.535	-1.972	1.00 44.73	Α
	MOTA	246 H	LEU	172	27.131	95.289	-1.448	1.00 0.00	A
20	MOTA	247 C		172	28.658	94.480	-2.675	1.00 43.36	A
	MOTA	248 C		172	28.434	93.125	-1.985	1.00 37.47	A
	MOTA	249 C		172	29.574	92.102	-1.869	1.00 35.42 1.00 32.59	A A
	ATOM		D1 LEU	172	29.011 30.274	90.764 91.926	-1.398 -3.189	1.00 32.89	A
25	ATOM		D2 LEU	$\frac{172}{172}$	28.214	94.362	-4.122	1.00 43.76	A
25	ATOM ATOM	252 C 253 O		172	29.013	94.070	-5.011	1.00 42.82	A
	ATOM	254 N		173	26.928	94.587	-4.345	1.00 45.41	A
	ATOM	255 H		173	26.349	94.834	-3.595	1.00 0.00	A
	MOTA		A LEU	173	26.354	94.481	-5.674	1.00 49.41	A
30	ATOM		B LEU	173	24.837	94.308	-5.561	1.00 52.76	A
	ATOM	258 C	G LEU	173	24.329	92.938	-5.089	1.00 54.19	A
	MOTA		D1 LEU	173	24.148	92.038	-6.294	1.00 59.26	A
	MOTA		D2 LEU	173	25.302	92.305	-4.110	1.00 54.13	A
0.5	MOTA	261 C		173	26.681	95.681	-6.552	1.00 51.49 1.00 46.63	A A
35	MOTA	262 0		173	27.079 26.523	95.521 96.882	-7.708 -5.997	1.00 40.03	A
	MOTA	263 N		174 174	26.220	96.946	-5.068	1.00 0.00	A
	ATOM ATOM	264 H 265 C	LYS A LYS	174	26.794	98.096	-6.751	1.00 51.25	A
	ATOM		B LYS	174	26.615	99.330	-5.862	1.00 50.79	Α
40	ATOM		G LYS	174	27.294	99.251	-4.513	1.00 49.59	A
	MOTA		D LYS	174	26.659	100.247	-3.542	1.00 48.26	A
	MOTA	269 C	E LYS	174		100.970	-2.714	1.00 41.18	A
	MOTA		IZ LYS	174		101.644	-3.574	1.00 37.27	A
	MOTA		IZ1 LYS	174		102.341	-4.183	1.00 0.00	A A
45	ATOM		IZ2 LYS	174		100.937 102.127	-4.168 -2.977	1.00 0.00 1.00 0.00	A
	MOTA	273 H 274 C	IZ3 LYS LYS	174 174	28.181	98.114	-7.384	1.00 48.99	A
	ATOM ATOM	274 C		174	28.439	98.906	-8.276	1.00 49.73	A
	ATOM	276 N		175	29.066		-6.928	1.00 51.76	A
50	ATOM	277 H		175	28.807	96.620	-6.212	1.00 0.00	A
-	MOTA		CA ARG	175	30.422	97.174	-7.471	1.00 54.88	A
	MOTA	279 C	B ARG	175	31.400	96.730	-6.378	1.00 60.59	A
	MOTA	280 C	CG ARG	175	32.257	97.853	-5.813	1.00 69.97	A
	MOTA		D ARG	175	32.030	98.026	-4.320	1.00 76.88	A
55	ATOM		NE ARG	175	32.502	99.320	-3.832	1.00 82.84	A A
	ATOM		HE ARG	175	33.238 31.996	99.324	-3.186 -4.208	1.00 0.00 1.00 86.91	A
	ATOM		Z ARG NH1 ARG	175 175	30.996		-5.080	1.00 88.00	A
	ATOM ATOM		HII ARG	175	30.620	99.687	-5.452	1.00 0.00	A
60	ATOM		H12 ARG	175	30.617		-5.361	1.00 0.00	A
00	ATOM		VH2 ARG	175		101.619	-3.712	1.00 88.60	A
	ATOM		121 ARG	175	33.245	101.588	-3.054	1.00 0.00	A
	MOTA	290 HF	122 ARG	175	32.112	102.499	-3.996	1.00 0.00	A
	MOTA	291 (	C ARG	175	30.543	96.231	-8.675	1.00 52.71	A
65	MOTA	292 (	) ARG	175	31.308	96.486	-9.604	1.00 51.98	A
	ATOM		N MET	176	29.777	95.147	-8.654	1.00 49.83	A
	MOTA		H MET	176	29.175	95.007	-7.894	1.00 0.00	A
	MOTA		CA MET	176	29.805	94.159	-9.720	1.00 44.82 1.00 39.16	A A
70	ATOM		CB MET	176	29.033	92.907	-9.306 -7.956	1.00 39.16	A A
70	ATOM		CG MET	176 176	29.372 28.290	92.339 90.955	-7.596 -7.596	1.00 37.27	A
	ATOM		SD MET CE MET	176	29.105	90.252	-6.182	1.00 36.51	A
	ATOM ATOM		C MET	176	29.208		-11.028	1.00 47.84	A
	521 OLI	500							

	MOTA	301	O MET	176	28.361	95.542 -11.049	1.00 46.58	A
	ATOM	302	N ASP	177	29.656	94.035 -12.118	1.00 51.49	A
	ATOM	303	H ASP	177	30.352	93.353 -12.016	1.00 0.00	A
	ATOM	304	CA ASP	177	29.157	94.329 -13.457	1.00 54.36	A
5	MOTA	305	CB ASP	177	30.322	94.519 -14.441	1.00 56.10	A
	MOTA	306	CG ASP	177	30.746	95.974 -14.586	1.00 60.14	A
	MOTA	307	OD1 ASP	177	31.960	96.219 -14.732	1.00 58.72	A
	MOTA	308	OD2 ASP	177	29.874	96.868 -14.559	1.00 61.23	A
	MOTA	309	C ASP	177	28.366	93.070 -13.833	1.00 54.37	A
10	ATOM	310	O ASP	177	28.944	92.089 -14.304	1.00 54.71	A
	ATOM	311	N ILE	178	27.056	93.088 -13.603	1.00 50.87	A
	ATOM	312	H ILE	178	26.644	93.892 -13.226	1.00 0.00	A
	ATOM	313	CA ILE	178	26.220	91.929 -13.905	1.00 50.24	A.
1 =	ATOM	314	CB ILE	178	24.921	91.933 -13.041	1.00 49.66 1.00 49.10	A A
15	ATOM	315	CG2 ILE	178	24.214 $25.275$	90.581 -13.131 92.217 -11.576	1.00 49.10	A
	ATOM	316	CG1 ILE CD1 ILE	178 178	24.125	92.001 -10.593	1.00 52.23	Ā
	ATOM ATOM	317 318	CDI ILE	178	25.855	91.871 -15.386	1.00 48.57	A
	MOTA	319	O ILE	178	25.743	92.905 -16.040	1.00 50.81	A
20	ATOM	320	N GLY	179	25.689	90.654 -15.902	1.00 48.26	A
20	ATOM	321	H GLY	179	25.801	89.873 -15.324	1.00 0.00	A
	ATOM	322	CA GLY	179	25.341	90.453 -17.300	1.00 47.18	A
	MOTA	323	C GLY	179	25.483	88.993 -17.708	1.00 47.42	A
	ATOM	324	O GLY	179	26.366	88.302 -17.203	1.00 44.46	A
25	ATOM	325	N PRO	180	24.635	88.489 -18.621	1.00 48.62	A
	ATOM	326	CD PRO	180	23.543	89.194 -19.313	1.00 50.81	A
	MOTA	327	CA PRO	180	24.730	87.084 -19.046	1.00 49.53	A
	MOTA	328	CB PRO	180	23.635	86.946 -20.107	1.00 48.70	A
	ATOM	329	CG PRO	180	22.692	88.070 -19.837	1.00 52.71	A
30	MOTA	330	C PRO	180	26.104	86.712 -19.597	1.00 52.68	A
	ATOM	331	O PRO	180	26.359	85.541 -19.902	1.00 53.20 1.00 49.61	A A
	ATOM	332	N LYS	181	26.983 26.720	87.706 -19.716 88.610 -19.445	1.00 49.81	A
	ATOM	333	H LYS	181 181	28.324	87.485 -20.238	1.00 49.94	A
35	MOTA MOTA	334 335	CA LYS CB LYS	181	28.517	88.279 -21.535	1.00 52.40	Ā
33	ATOM	336	CG LYS	181	27.413	88.064 -22.577	1.00 52.89	A
	ATOM	337	CD LYS	181	27.111	86.588 -22.801	1.00 50.48	A
	ATOM	338	CE LYS	181	28.125	85.942 -23.735	1.00 54.32	A
	ATOM	339	NZ LYS	181	29.156	85.176 -22.981	1.00 54.02	A
40	ATOM	340	HZ1 LYS	181	28.696	84.425 -22.427	1.00 0.00	A
-	ATOM	341	HZ2 LYS	181	29.664	85.818 -22.338	1.00 0.00	A
	MOTA	342	HZ3 LYS	181	29.830	84.750 -23.648	1.00 0.00	A
	MOTA	343	C LYS	181	29.389	87.882 -19.223	1.00 49.03	A
	MOTA	344	O LYS	181	30.575	87.943 -19.544	1.00 44.77	A
45	MOTA	345	N GLN	182	28.953	88.150 -17.997	1.00 49.13	A
	ATOM	346	H GLN	182	27.997	88.071 -17.806	1.00 0.00	A
	ATOM	347	CA GLN	182	29.855	88.549 -16.927 89.802 -17.332	1.00 47.58 1.00 52.30	A A
	ATOM	348	CB GLN	182	30.657	91.148 -17.105	1.00 52.30	A
50	MOTA	349	CG GLN	182 182	29.961 29.400	91.760 -18.381	1.00 59.68	A
50	ATOM ATOM	350 351	CD GLN OE1 GLN	182	28.651	92.742 -18.337	1.00 59.75	A
	ATOM	352	NE2 GLN	182	29.759	91.184 -19.526	1.00 62.02	A
	ATOM		HE21 GLN	182	30.356	90.408 -19.515	1.00 0.00	A
	ATOM		HE22 GLN	182	29.407	91.567 -20.355	1.00 0.00	A
55	ATOM	355	C GLN	182	29.039	88.817 -15.673	1.00 46.05	A
	ATOM	356	O GLN	182	28.205	89.720 -15.635	1.00 52.56	A
	ATOM	357	N THR	183	29.279	88.007 -14.655	1.00 43.42	A
	MOTA	358	H THR	183	29.952	87.304 -14.768	1.00 0.00	A
	MOTA	359	CA THR	183	28.590	88.107 -13.367	1.00 39.86	A
60	MOTA	360	CB THR	183	28.994	89.369 -12.571	1.00 38.78	A
	MOTA	361	OG1 THR	183	30.422	89.443 -12.473	1.00 33.64	A
	MOTA	362	HG1 THR	183	30.753	88.664 -12.022	1.00 0.00	A
	ATOM	363	CG2 THR	183	28.407	89.303 -11.165 88.054 -13.388	1.00 36.70 1.00 40.16	A A
65	ATOM	364	C THR	183 183	27.073 26.397	88.889 -14.001	1.00 40.10	Ā
65	MOTA	365	O THR	184	26.565	87.044 -12.692	1.00 37.02	A
	ATOM	366	N GLN	184	27.185	86.424 -12.260	1.00 0.00	A
	MOTA MOTA	367 368	H GLN CA GLN	184	25.148	86.805 -12.534	1.00 32.70	A
	ATOM	369	CB GLN	184	24.755	85.500 -13.199	1.00 39.22	A
70	ATOM	370	CG GLN	184	24.950	85.502 -14.684	1.00 38.77	A
, 0	ATOM	371	CD GLN	184	23.866	84.736 -15.379	1.00 37.99	A
	ATOM	372	OE1 GLN	184	23.633	83.563 -15.081	1.00 34.86	A
	ATOM	373	NE2 GLN	184	23.182	85.395 -16.306	1.00 36.73	A

	ATOM		HE21 GLN	184	23.400		-16.503	1.00 0.00	A
	ATOM		HE22 GLN	184	22.470		-16.770	1.00 0.00 1.00 34.89	A A
	ATOM	376	C GLN	184 184	24.956 25.816		-11.032 -10.331	1.00 34.69	A
5	ATOM ATOM	377 378	O GLN N VAL	185	23.819		-10.552	1.00 35.52	A
5	ATOM	379	H VAL	185	23.168	87.567	-11.175	1.00 0.00	A
	MOTA	380	CA VAL	185	23.510	87.179	-9.129	1.00 33.81	A
	MOTA	381	CB VAL	185	23.602	88.617	-8.545	1.00 35.05	A
10	ATOM	382	CG1 VAL	185	23.088	88.636	-7.094	1.00 35.71 1.00 16.86	A A
10	ATOM	383	CG2 VAL C VAL	185 185	25.048 22.137	89.115 86.604	-8.612 -8.772	1.00 10.86	A
	ATOM ATOM	384 385	C VAL O VAL	185	21.129	86.859	-9.441	1.00 29.48	A
	ATOM	386	N GLY	186	22.129	85.830	-7.691	1.00 29.37	A
	ATOM	387	H GLY	186	22.968	85.675	-7.209	1.00 0.00	A
15	MOTA	388	CA GLY	186	20.915	85.215	-7.208	1.00 33.55	A
	ATOM	389	C GLY	186 186	20.922 21.978	85.345 85.507	-5.706 -5.092	1.00 30.62 1.00 38.55	A A
	ATOM ATOM	390 391	O GLY N ILE	187	19.751	85.285	-5.100	1.00 29.16	A
	MOTA	392	H ILE	187	18.935	85.152	-5.626	1.00 0.00	A
20	MOTA	393	CA ILE	187	19.667	85.411	-3.657	1.00 29.27	A
	MOTA	394	CB ILE	187	19.244	86.832	-3.222	1.00 23.80	A A
	ATOM	395	CG2 ILE CG1 ILE	187 187	19.187 20.223	86.902 87.869	-1.708 -3.771	1.00 21.78 1.00 25.79	A
	ATOM ATOM	396 397	CD1 ILE	187	20.020	89.264	-3.200	1.00 26.87	A
25	ATOM	398	C ILE	187	18.656	84.456	-3.063	1.00 28.09	A
	MOTA	399	O ILE	187	17.537	84.337	-3.549	1.00 26.92	A
	MOTA	400	N VAL	188	19.057	83.793	-1.989	1.00 31.92 1.00 0.00	A A
	ATOM ATOM	401 402	H VAL CA VAL	188 188	19.971 18.175	83.924 82.877	-1.660 -1.288	1.00 31.88	A
30	ATOM	402	CB VAL	188	18.598	81.408	-1.538	1.00 30.39	A
20	ATOM	404	CG1 VAL	188	18.918	80.702	-0.221	1.00 23.72	A
	ATOM	405	CG2 VAL	188	17.478	80.688	-2.276	1.00 31.57	A
	ATOM	406	C VAL	188 188	18.271 19.362	83.226 83.436	0.198 0.719	1.00 30.17 1.00 29.85	A A
35	ATOM ATOM	407 408	O VAL N GLN	189	17.132	83.332	0.869	1.00 26.31	A
33	ATOM	409	H GLN	189	16.278	83.201	0.405	1.00 0.00	A
	ATOM	410	CA GLN	189	17.146	83.644	2.288	1.00 27.42	A
	ATOM	411	CB GLN	189	16.219	84.830	2.629	1.00 25.02 1.00 21.62	A A
40	ATOM ATOM	412 413	CG GLN CD GLN	189 189	16.196 15.631	85.140 86.506	$4.141 \\ 4.495$	1.00 21.62	A
40	ATOM	414	OE1 GLN	189	15.554	86.867	5.668	1.00 23.48	A
	ATOM	415	NE2 GLN	189	15.230	87.263	3.487	1.00 26.01	A
	MOTA		HE21 GLN	189	15.304	86.940	2.567	1.00 0.00	A
15	MOTA		HE22 GLN	189	14.866 16.679	88.147 82.392	3.709 3.000	1.00 0.00 1.00 23.00	A A
45	MOTA ATOM	418 419	C GLN O GLN	189 189	15.882	81.631	2.463	1.00 23.43	A
	ATOM	420	N TYR	190	17.184	82.171	4.202	1.00 22.53	A
	ATOM	421	H TYR	190	17.820	82.811	4.584	1.00 0.00	A
<b>~</b> 0	ATOM	422	CA TYR	190	16.811	80.993		1.00 26.52 1.00 26.90	A
50	ATOM ATOM	423 424	CB TYR CG TYR	190 190	17.837 19.147	79.883 80.113		1.00 28.90	A A
	ATOM	425	CD1 TYR	190	19.397	79.503		1.00 15.45	A
	ATOM	426	CE1 TYR	190	20.593	79.699		1.00 17.09	A
	MOTA	427	CD2 TYR	190	20.139	80.936		1.00 14.28	A
55	MOTA	428	CE2 TYR	190	21.347 21.567	81.138 80.513		1.00 14.48 1.00 15.88	A A
	MOTA MOTA	429 430	CZ TYR OH TYR	190 190	22.749	80.701		1.00 15.41	A
	MOTA	431	HH TYR	190	23.313	81.297		1.00 0.00	A
	MOTA	432	C TYR	190	16.694	81.265		1.00 28.88	A
60	MOTA	433	O TYR	190	17.147	82.297		1.00 27.66	A
	ATOM	434	N GLY	191	16.093 15.773	80.302 79.511		1.00 29.28 1.00 0.00	A A
	ATOM ATOM	435 436	H GLY CA GLY	191 191	15.773	80.359		1.00 26.48	A
	ATOM	437	C GLY	191	14.655	79.507		1.00 27.88	A
65	ATOM	438	O GLY	191	13.548	79.953		1.00 33.37	A
	MOTA	439	N GLU	192	14.843	78.283		1.00 31.94	A
	ATOM	440	H GLU	192	15.753 13.744	78.004 77.334		1.00 0.00 1.00 34.41	A A
	MOTA MOTA	$\frac{441}{442}$	CA GLU CB GLU	192 192	13.744	78.026		1.00 34.41	A
70	ATOM	443	CG GLU	192	12.439	78.147		1.00 39.53	A
. •	ATOM	444	CD GLU	192	11.319	79.079	11.967	1.00 39.25	A
	MOTA	445	OE1 GLU	192	11.611	80.085	12.645	1.00 42.52	A A
	MOTA	446	OE2 GLU	192	10.146	78.813	11.616	1.00 34.89	А

	ATOM	447 C	GLU	192	13.384	76.697	8.111	1.00 34.47	A
			GLU	192	13.208	75.487	8.010	1.00 36.09	A
	ATOM							1.00 33.33	A
	ATOM	449 N	ASN	193	13.265	77.528	7.082		
	MOTA	450 H	ASN	193	13.403	78.487	7.234	1.00 0.00	A
5	ATOM	451 CZ	A ASN	193	12.935	77.071	5.736	1.00 35.22	A
	ATOM	452 CI	B ASN	193	11.409	77.105	5.534	1.00 38.44	A
	ATOM	453 CC		193	10.967	78.108	4.484	1.00 42.52	A
	ATOM		D1 ASN	193	10.607	77.735	3.366	1.00 48.03	A
				193	10.987	79.383	4.840	1.00 45.99	A
10	MOTA		D2 ASN						A
10	MOTA	456 HD2		193	11.275	79.633	5.739		
	MOTA	457 HD2	22 ASN	193	10.705	80.040	4.172	1.00 0.00	A
	ATOM	458 C	ASN	193	13.674	77.964	4.718	1.00 31.48	A
	ATOM	459 O	ASN	193	14.389	78.885	5.114	1.00 32.85	A
	MOTA	460 N	VAL	194	13.516	77.699	3.423	1.00 28.41	A
15	ATOM	461 H		194	12.921	76.971	3.148	1.00 0.00	A
13					14.216	78.485	2.408	1.00 30.39	A
	ATOM	462 C		194				1.00 35.86	A
	ATOM	463 CI		194	15.300	77.621	1.682		
	MOTA	464 C	G1 VAL	194	16.253	78.517	0.890	1.00 34.87	A
	ATOM	465 C	G2 VAL	194	16.086	76.798	2.700	1.00 31.70	A
20	ATOM	466 C	VAL	194	13.312	79.100	1.347	1.00 26.35	A
	ATOM	467 0	VAL	194	12.352	78.487	0.911	1.00 25.27	A
	ATOM	468 N		195	13.629	80.327	0.938	1.00 30.82	A
				195	14.396	80.780	1.344	1.00 0.00	A
	ATOM	469 H							
	ATOM	470 C		195	12.861	81.013	-0.097	1.00 32.80	A
25	ATOM	471 C		195	11.875	82.059	0.520	1.00 32.61	A
	ATOM	472 0	G1 THR	195	12.435	83.370	0.439	1.00 36.07	A
	ATOM	473 H	G1 THR	195	11.821	84.005	0.819	1.00 0.00	A
	ATOM		G2 THR	195	11.581	81.730	1.969	1.00 35.80	A
	ATOM	475 C		195	13.832	81.698	-1.066	1.00 34.36	A
30				195	14.830	82.274	-0.638	1.00 37.20	A
30	ATOM	476 0					-2.368	1.00 37.20	A
	MOTA	477 N		196	13.562	81.610			
	ATOM	478 H	HIS	196	12.767	81.117	-2.664	1.00 0.00	A
	MOTA	479 C.	A HIS	196	14.430	82.235	-3.364	1.00 33.42	A
	ATOM	480 C	B HIS	196	14.373	81.488	-4.703	1.00 36.34	A
35	ATOM	481 C	G HIS	196	14.682	80.027	-4.612	1.00 32.56	A
	ATOM		D2 HIS	196	13.920	78.975	-4.231	1.00 33.30	A
	ATOM		D1 HIS	196	15.885	79.493	-5.025	1.00 30.72	A
				196	16.646	80.005	-5.357	1.00 0.00	A
	MOTA		D1 HIS					1.00 27.16	A
4.0	ATOM		E1 HIS	196	15.850	78.181	-4.905		
40	ATOM		E2 HIS	196	14.669	77.839	-4.425	1.00 24.32	A
	MOTA	487 H	E2 HIS	196	14.366	76.932	-4.234	1.00 0.00	A
	ATOM	488 C	HIS	196	13.990	83.676	-3.600	1.00 33.69	A
	ATOM	489 O	HIS	196	12.907	83.910	-4.147	1.00 30.28	A
	ATOM	490 N		197	14.825	84.633	-3.193	1.00 32.40	A
45	ATOM	491 H		197	15.670	84.376	-2.769	1.00 0.00	A
45					14.522	86.053	-3.357	1.00 28.21	A
	MOTA			197					
	MOTA		B GLU	197	15.485	86.884	-2.515	1.00 30.79	A
	MOTA	494 C	G GLU	197	15.369	86.601	-1.025	1.00 29.25	A
	MOTA	495 C	D GLU	197	13.980	86.880	-0.489	1.00 28.81	A
50	MOTA	496 O	E1 GLU	197	13.154	87.429	-1.246	1.00 27.20	A
	MOTA		E2 GLU	197	13.712	86.550	0.688	1.00 31.09	A
	ATOM	498 C		197	14.578	86.469	-4.831	1.00 25.47	A
		499 0		197	13.872	87.380	-5.250	1.00 33.41	A
	ATOM							1.00 28.05	A
	MOTA	500 N		198	15.447	85.817	-5.594		
55	MOTA	501 H		198	16.035	85.161	-5.166	1.00 0.00	A
	ATOM	502 C	A PHE	198	15.573	86.023	-7.038	1.00 29.94	A
	MOTA	503 C	B PHE	198	15.668	87.522	-7.420	1.00 22.28	A
	ATOM		G PHE	198	16.939	88.213	-7.021	1.00 20.44	A
	ATOM		D1 PHE	198	18.134	87.969	-7.696	1.00 29.59	A
60			D2 PHE	198	16.925	89.166	-6.015	1.00 12.83	A
oo	ATOM					88.669	-7.376	1.00 23.18	A
	MOTA		E1 PHE	198	19.300				
	MOTA		E2 PHE	198	18.074	89.872	-5.683	1.00 23.57	A
	MOTA	509 C	Z PHE	198	19.269	89.626	-6.364	1.00 26.69	A
	MOTA	510 C	PHE	198	16.684	85.181	-7.679	1.00 34.58	A
65	ATOM	511 0		198	17.787	85.048	-7.131	1.00 35.32	A
	MOTA	512 N		199	16.352	84.590	-8.828	1.00 33.63	A
				199	15.456	84.756	-9.187	1.00 0.00	A
	ATOM					83.708	-9.592	1.00 33.60	A
	MOTA		A ASN	199	17.237				
	MOTA		B ASN	199	16.416	82.890	-10.596	1.00 33.43	A
70	MOTA	516 C	G ASN	199	15.406	81.979	-9.929	1.00 35.08	A
	MOTA		D1 ASN	199	15.458	81.743	-8.724	1.00 37.14	А
	ATOM		ID2 ASN	199	14.480		-10.717	1.00 36.96	A
	MOTA		21 ASN	199	14.477		-11.674	1.00 0.00	A
	111 Ori	J = J = 111							-

	ATOM	520 F	HD22	ASN	199	13.818	80.865	-10.306	1.00 0.00	A
	ATOM	521		ASN	199	18.381	84.392	-10.352	1.00 37.18	A
	ATOM	522	0 2	ASN	199	18.312	85.573	-10.690	1.00 33.75	A
	ATOM	523	N :	LEU	200	19.413	83.605		1.00 35.28	A
5	MOTA	524	Н :	LEU	200	19.374	82.663		1.00 0.00	A
	MOTA	525		LEU	200	20.595	84.080		1.00 36.97	A
	ATOM	526		LEU	200	21.612	82.943		1.00 36.01	A
	ATOM	527		LEU	200	22.358	82.306		1.00 32.50	A
	ATOM	528	CD1		200	21.430	81.966	-9.168	1.00 38.36	A
10	ATOM	529	CD2		200	22.997	81.034		1.00 33.04	A
	ATOM	530		LEU	200	20.304	84.640		1.00 36.89	A A
	ATOM	531		LEU	200	21.069		-13.256	1.00 38.59 1.00 38.74	A
	MOTA	532		ASN	201	19.217		-13.370 -12.929	1.00 38.74	A
15	MOTA	533		ASN	201	18.633 18.891		-12.929 $-14.713$	1.00 40.95	A
15	ATOM	534		ASN ASN	201 201	18.643		-15.666	1.00 42.74	A
	ATOM ATOM	535 536		asn Asn	201	17.424		-15.284	1.00 45.08	A
	ATOM	537	OD1		201	17.100		-15.969	1.00 46.68	A
	ATOM	538	ND2		201	16.746		-14.199	1.00 42.33	A
20	ATOM		HD21		201	17.038		-13.682	1.00 0.00	A
20	ATOM		HD22		201	15.963		-13.952	1.00 0.00	A
	ATOM	541		ASN	201	17.696	85.616	-14.726	1.00 41.99	A
	ATOM	542		ASN	201	17.194	85.997	-15.785	1.00 36.95	A
	MOTA	543	N	LYS	202	17.257		-13.532	1.00 43.02	A
25	ATOM	544	H	LYS	202	17.711	85.657	-12.731	1.00 0.00	A
	MOTA	545	CA	LYS	202	16.127		-13.378	1.00 42.25	A
	MOTA	546	CB	LYS	202	15.743		-11.896	1.00 37.84	A
	ATOM	547	CG	LYS	202	14.984		-11.505	1.00 39.09	A
	$\mathbf{MOTA}$	548		LYS	202	13.486		-11.664	1.00 41.90	A
30	MOTA	549		LYS	202	12.851		-10.381	1.00 47.46	A
	ATOM	550		LYS	202	12.961		-10.253	1.00 45.02 1.00 0.00	A A
	MOTA	551	HZ1		202	13.963		-10.250 $-11.057$	1.00 0.00	A
	ATOM	552 552	HZ2		202 202	12.479 $12.513$	85.699	-9.366	1.00 0.00	A
35	ATOM	553 554	HZ3	LYS	202	16.443		-13.921	1.00 40.53	A
33	ATOM ATOM	555		LYS	202	15.698		-14.735	1.00 36.63	A
	ATOM	556		TYR	203	17.558		-13.486	1.00 41.00	A
	ATOM	557		TYR	203	18.140		-12.861	1.00 0.00	A
	ATOM	558		TYR	203	17.923		-13.931	1.00 40.78	A
40	ATOM	559	CB	TYR	203	18.101	91.114	-12.711	1.00 43.99	A
	ATOM	560	CG	TYR	203	16.946	91.108	-11.723	1.00 42.62	A
	MOTA	561	CD1	TYR	203	17.064		-10.483	1.00 42.17	A
	MOTA	562	CE1	TYR	203	16.027	90.492	-9.556	1.00 36.22	A
	MOTA	563	CD2		203	15.750		-12.010	1.00 44.83	A
45	MOTA	564		TYR	203	14.702	91.786	-11.086	1.00 48.25	A
	MOTA	565	CZ	TYR	203	14.848	91.151	-9.860	1.00 47.45 1.00 52.58	A A
	ATOM	566	OH	TYR	203	13.815	91.181 91.678	-8.942 -9.304	1.00 32.38	A
	ATOM	567	HH	TYR	203	13.077 19.181		-14.813	1.00 42.72	A
50	ATOM	568 560	C	TYR	203 203	20.014	20.243	-14.784	1.00 38.83	A
50	ATOM ATOM	569 570	O N	TYR SER	203	19.313	91 312	-15.591	1.00 43.42	A
	ATOM	571	H	SER	204	18.628	92.013	-15.556	1.00 0.00	A
	ATOM	572	CA	SER	204	20.445		-16.499	1.00 45.46	A
	ATOM	573	CB	SER	204	19.945	91.613	-17.933	1.00 47.15	A
55	ATOM	574	ŌĠ	SER	204	19.893	92.982	-18.309	1.00 49.62	A
	MOTA	575	$^{\mathrm{HG}}$	SER	204	20.770		-18.244	1.00 0.00	A
	MOTA	576	C	SER	204	21.312	92.691	-16.188	1.00 49.08	A
	MOTA	577	0	SER	204	22.464		-16.616	1.00 48.50	A
	MOTA	578	N	SER	205	20.757		-15.462	1.00 50.50	A
60	ATOM	579	H	SER	205	19.839		-15.138	1.00 0.00	A
	ATOM	580	CA	SER	205	21.495		-15.141	1.00 49.60	A
	MOTA	581	CB	SER	205	20.634	96.098	-15.449	1.00 49.35	A
	ATOM	582	OG	SER	205	21.303		-16.345	1.00 54.35	A
	MOTA	583	HG	SER	205	22.128		-15.950	1.00 0.00 1.00 47.82	A A
65	ATOM	584	C	SER	205	21.981		-13.699	1.00 47.82	A
	MOTA	585	0	SER	205	21.316		-12.785 -13.512	1.00 41.96	A
	MOTA	586	N	THR	206	23.151 23.643		-13.512 $-14.287$	1.00 48.13	A
	MOTA	587	H	THR	206	23.643		-14.267 $-12.184$	1.00 49.52	A
70	MOTA	588	CA	THR THR	206 206	25.121	96 351	-12.104	1.00 46.33	A
70	MOTA MOTA	589 590	CB OG1	THR	206	26.115		-12.233	1.00 47.49	A
	ATOM	591		THR	206	26.050		-11.545	1.00 0.00	A
	ATOM	592		THR	206	25.381		-10.980	1.00 46.12	A
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	ATOM	593	С	THR	206	22.792	96.617	-11.383	1.00 49.12	A
	ATOM	594	Ö	THR	206	22.684		-10.166	1.00 53.03	A
	ATOM	595	N	GLU	207	22.123		-12.070	1.00 51.42	A
									1.00 0.00	A
_	MOTA	596	H	GLU	207	22.243		-13.042		
5	ATOM	597	CA	GLU	207	21.215		-11.408	1.00 49.16	A
	ATOM	598	CB	GLU	207	21.002		-12.269	1.00 52.87	A
	ATOM	599	CG	GLU	207	21.187	99.521	-13.762	1.00 55.52	A
	ATOM	600	CD	GLU	207	20.886	100.782	-14.550	1.00 56.44	A
	ATOM	601	OE1		207		101.489		1.00 55.48	A
10				GLU	207		101.066		1.00 53.55	A
10	ATOM	602								A
	MOTA	603	C	GLU	207	19.864		-11.066	1.00 49.23	
	$\mathtt{MOTA}$	604	0	GLU	207	19.350	98.053	-9.964	1.00 48.23	A
	MOTA	605	N	GLU	208	19.276		-12.000	1.00 47.83	A
	ATOM	606	H	GLU	208	19.710	96.988	-12.870	1.00 0.00	A
15	ATOM	607	CA	GLU	208	17.981	96.511	-11.727	1.00 48.69	A
	ATOM	608	CB	GLU	208	17.500	95.700	-12.916	1.00 45.35	A
	ATOM	609	CG	GLU	208	17.020		-14.082	1.00 40.10	A
					208	16.724		-15.262	1.00 37.99	A
	ATOM	610	CD	GLU						A
••	ATOM	611	OE1		208	15.676		-15.918	1.00 46.28	
20	MOTA	612	OE2	GLU	208	17.545		-15.528	1.00 36.45	A
	MOTA	613	С	GLU	208	18.129		-10.535	1.00 50.21	A
	ATOM	614	0	GLU	208	17.317	95.603	-9.608	1.00 50.81	A
	ATOM	615	N	VAL	209	19.174	94.764	-10.573	1.00 47.53	A
	ATOM	616	Н	VAL	209	19.778	94.788	-11.344	1.00 0.00	A
25	MOTA	617	CA	VAL	209	19.436	93.832	-9.489	1.00 48.06	A
23			CB	VAL	209	20.744	93.024	-9.738	1.00 48.35	A
	ATOM	618						-8.421		
	MOTA	619	CG1		209	21.363	92.582		1.00 49.78	A
	MOTA	620	CG2		209	20.446	91.809	-10.589	1.00 49.88	A
	ATOM	621	C	VAL	209	19.549	94.619	-8.187	1.00 45.25	A
30	ATOM	622	0	VAL	209	19.145	94.138	-7.134	1.00 43.45	A
	ATOM	623	N	LEU	210	20.081	95.836	-8.263	1.00 45.57	A
	ATOM	624	H	LEU	210	20.373	96.189	-9.130	1.00 0.00	A
	ATOM	625	CA	LEU	210	20.232	96.652	-7.061	1.00 46.10	A
						21.031	97.931	-7.356	1.00 44.07	A
25	ATOM	626	CB	LEU	210					
35	MOTA	627	CG	LEU	210	22.557	97.828	-7.549	1.00 44.26	A
	ATOM	628		LEU	210	23.131	99.226	-7.738	1.00 38.37	A
	ATOM	629	CD2	LEU	210	23.218	97.138	-6.361	1.00 35.26	A
	MOTA	630	C	LEU	210	18.862	97.006	-6.490	1.00 44.20	A
	ATOM	631	0	LEU	210	18.653	96.925	-5.286	1.00 44.77	A
40	ATOM	632	N	VAL	211	17.928	97.389	-7.349	1.00 45.51	A
	ATOM	633	H	VAL	211	18.137	97.445	-8.305	1.00 0.00	A
		634	CA	VAL	211	16.591	97.731	-6.880	1.00 44.84	A
	ATOM								1.00 44.98	A
	ATOM	635	CB	VAL	211	15.685	98.253	-8.021		
	ATOM	636	CG1		211	14.649	99.213	-7.449	1.00 49.23	A
45	ATOM	637	CG2	VAL	211	16.517	98.940	-9.095	1.00 47.62	A
	ATOM	638	C	VAL	211	15.914	96.503	-6.278	1.00 42.72	A
	ATOM	639	0	VAL	211	15.219	96.595	-5.262	1.00 42.50	A
	ATOM	640	N	ALA	212	16.122	95.353	-6.907	1.00 40.62	Α
	ATOM	641	Н	ALA	212	16.699	95.334	-7.699	1.00 0.00	A
50	ATOM	642	CA	ALA	212	15.509	94.116	-6.440	1.00 40.77	A
50			CB	ALA	212	15.742	93.011	-7.454	1.00 36.33	A
	MOTA	643					93.672	-5.063	1.00 38.58	A
	ATOM	644	C	ALA	212	16.001				
	ATOM	645	0	ALA	212	15.207	93.243	-4.221	1.00 37.62	A
	ATOM	646	N	ALA	213	17.305	93.779	-4.837	1.00 31.59	A
55	ATOM	647	H	ALA	213	17.889	94.145	-5.532	1.00 0.00	A
	MOTA	648	CA	ALA	213	17.879	93.359	-3.564	1.00 35.24	A
	ATOM	649	CB	ALA	213	19.386	93.229	-3.687	1.00 35.74	A
	ATOM	650	c	ALA	213	17.540	94.277	-2.404	1.00 33.73	A
				ALA	213	17.515	93.837	-1.264	1.00 30.39	A
60	MOTA	651	0						1.00 37.82	A
60	MOTA	652	N	ASN	214	17.277	95.548	-2.688		
	ATOM	653	H	ASN	214	17.292	95.854	-3.618	1.00 0.00	A
	MOTA	654	$^{\rm CA}$	ASN	214	16.962	96.495	-1.620	1.00 41.93	A
	ATOM	655	CB	ASN	214	17.152	97.935	-2.102	1.00 43.82	A
	ATOM	656	CG	ASN	214	18.495	98.509	-1.688	1.00 45.59	A
65	MOTA	657		ASN	214	19.426	98.581	-2.492	1.00 47.44	A
03	ATOM	658		ASN	214	18.606	98.911	-0.425	1.00 46.09	A
							98.829	0.183	1.00 40.03	A
	ATOM		HD21		214	17.842				
	ATOM		HD22		214	19.465	99.284	-0.143	1.00 0.00	A
	ATOM	661	С	ASN	214	15.555	96.313	-1.084	1.00 44.23	A
70	MOTA	662	0	ASN	214	15.232	96.808	-0.009	1.00 45.11	A
	ATOM	663	N	LYS	215	14.724	95.589	-1.830	1.00 44.69	A
	MOTA	664	Н	LYS	215	15.045	95.212	-2.677	1.00 0.00	A
	MOTA	665	CA	LYS	215	13.351	95.347	-1.416	1.00 43.68	A
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	ATOM	666	СВ	LYS	215	12.425	95.401	-2.632	1.00 45.74	7\
	ATOM	667	CG	LYS	215	12.506	94.172	-3.524	1.00 43.74	A
	ATOM	668	CD	LYS	215	12.162	94.511	-3.524 $-4.971$	1.00 55.87	A
	ATOM	669	CE	LYS	215	11.845	93.258	-4.971 $-5.776$		A
5									1.00 59.40	A
3	MOTA	670	NZ	LYS	215	10.388	92.928	-5.762	1.00 58.33	A
	ATOM	671		LYS	215	9.850	93.718	-6.173	1.00 0.00	A
	ATOM	672	HZ2	LYS	215	10.077	92.768	-4.784	1.00 0.00	A
	MOTA	673	HZ3	LYS	215	10.223	92.068	-6.323	1.00 0.00	A
	ATOM	674	С	LYS	215	13.184	94.007	-0.701	1.00 41.09	A
10	MOTA	675	0	LYS	215	12.073	93.505	-0.575	1.00 41.46	Α
	MOTA	676	N	ILE	216	14.280	93.427	-0.227	1.00 38.99	A
	MOTA	677	H	$_{ m ILE}$	216	15.151	93.863	-0.342	1.00 0.00	A
	ATOM	678	CA	ILE	216	14.197	92.146	0.463	1.00 34.14	A
	ATOM	679	CB	ILE	216	15.477	91.305	0.281	1.00 34.14	A
15	ATOM	680		ILE	216	15.367	90.029	1.102		
13									1.00 30.52	A
	ATOM	681		ILE	216	15.694	90.973	-1.192	1.00 29.14	A
	ATOM	682		ILE	216	17.084	90.443	-1.481	1.00 27.72	A
	ATOM	683	С	$_{ m ILE}$	216	13.987	92.335	1.952	1.00 31.56	A
	ATOM	684	0	$_{ m ILE}$	216	14.823	92.918	2.637	1.00 31.71	A
20	ATOM	685	N	GLY	217	12.874	91.824	2.458	1.00 33.70	A
	ATOM	686	H	GLY	217	12.242	91.354	1.875	1.00 0.00	A
	ATOM	687	CA	GLY	217	12.595	91.962	3.872	1.00 36.08	A
	ATOM	688	C	GLY	217	13.014	90.749	4.680	1.00 38.70	A
	MOTA	689	0	GLY	217	13.112	89.642	4.141	1.00 38.11	A
25	ATOM	690	N	ARG	218	13.269	90.965	5.968	1.00 37.58	A
	ATOM	691	H	ARG	218	13.193	91.876	6.318	1.00 37.38	
	ATOM	692	CA	ARG	218	13.667				A
							89.895	6.884	1.00 38.94	A
	ATOM	693	CB	ARG	218	13.990	90.473	8.267	1.00 37.57	A
20	ATOM	694	CG	ARG	218	14.512	89.462	9.295	1.00 40.84	A
30	ATOM	695	CD	ARG	218	15.880	89.885	9.830	1.00 43.84	A
	MOTA	696	NE	ARG	218	16.011	89.820	11.283	1.00 35.18	A
	MOTA	697	$_{ m HE}$	ARG	218	16.023	88.935	11.701	1.00 0.00	A
	MOTA	698	CZ	ARG	218	16.126	90.882	12.073	1.00 36.87	A
	ATOM	699	NH1	ARG	218	16.126	92.114	11.573	1.00 27.19	A
35	ATOM	700	HH11	ARG	218	16.055	92.253	10.583	1.00 0.00	A
	ATOM	701	HH12	ARG	218	16.212	92.903	12.181	1.00 0.00	A
	MOTA	702	NH2		218	16.263	90.706	13.374	1.00 41.63	A
	ATOM		HH21		218	16.287	89.785	13.753	1.00 0.00	A
	ATOM		HH22	ARG	218	16.345	91.499	13.979	1.00 0.00	A
40	ATOM	705	C	ARG	218	12.546	88.873	7.006	1.00 35.63	
40	ATOM	706		ARG	218	11.488	89.167			A
			0					7.556	1.00 43.27	A
	ATOM	707	N	GLN	219	12.788	87.667	6.504	1.00 39.56	A
	ATOM	708	H	GLN	219	13.661	87.489	6.097	1.00 0.00	A
45	MOTA	709	CA	GLN	219	11.792	86.602	6.541	1.00 38.70	A
45	MOTA	710	CB	GLN	219	12.265	85.411	5.694	1.00 33.61	A
	ATOM	711	CG	GLN	219	12.960	84.295	6.452	1.00 32.85	A
	ATOM	712	CD	GLN	219	12.950	82.995	5.682	1.00 33.39	A
	ATOM	713	OE1	GLN	219	12.946	82.990	4.449	1.00 38.03	A
	ATOM	714	NE2	GLN	219	12.938	81.883	6.402	1.00 39.97	A
50	ATOM	715	HE21	GLN	219	12.936	81.933	7.380	1.00 0.00	A
	ATOM			GLN	219	12.931	81.032	5.917	1.00 0.00	A
	MOTA	717	С	GLN	219	11.465	86.161	7.961	1.00 41.40	A
	MOTA	718	Ö	GLN	219	10.317	85.831	8.269	1.00 40.86	A
	MOTA	719	N	GLY	220	12.470	86.161	8.828	1.00 40.86	
55	ATOM	720	H	GLY	220	13.369	86.424	8.536	1.00 40.80	A
55	ATOM	721	CA		220					A
				GLY		12.241	85.771	10.206	1.00 40.81	A
	ATOM	722	C	GLY	220	12.464	84.299	10.470	1.00 41.52	A
	MOTA	723	0	GLY	220	12.137	83.447	9.650	1.00 37.96	A
<b>60</b>	MOTA	724	N	GLY	221	13.022	84.001	11.634	1.00 44.63	A
60	MOTA	725	H	GLY	221	13.258	84.716	12.260	1.00 0.00	A
	MOTA	726	CA	GLY	221	13.282	82.623	11.987	1.00 43.63	A
	MOTA	727	C	GLY	221	13.912	82.468	13.354	1.00 44.55	A
	MOTA	728	0	GLY	221	14.805	83.221	13.742	1.00 40.07	A
	ATOM	729	N	LEU	222	13.416	81.477	14.085	1.00 45.22	A
65	ATOM	730	H	LEU	222	12.691	80.940	13.711	1.00 0.00	A
	ATOM	731	CA	LEU	222	13.903	81.151	15.411	1.00 47.35	A
	ATOM	731	CB	LEU	222	12.781	80.471			
								16.207	1.00 54.79	A
	ATOM	733	CG CD1	LEU	222	11.395	80.687	15.579	0.01 54.77	A
70	ATOM	734	CD1		222	10.343	79.881	16.311	0.01 55.93	A
70	ATOM	735	CD2		222	11.048	82.171	15.608	0.01 57.10	A
	MOTA	736	С	LEU	222	15.066	80.194	15.172	1.00 47.02	A
	ATOM	737	0	LEU	222	16.135	80.340	15.757	1.00 47.47	A
	MOTA	738	N	GLN	223	14.837	79.233	14.279	1.00 42.82	A

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APOM		ATOM	754	OG1 TH	R 224	19.462	80.968	12.668	1.00 31.13	A
APOM		ATOM	755	HG1 TH	R 224	19.146	81.401	11.872	1.00 0.00	A
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ATOM 766 C MET 225 20.205 76.326 7.958 1.00 27.44 A 30 ATOM 767 O MET 225 19.850 76.238 6.785 1.00 27.44 A 30 ATOM 768 N THR 226 21.446 76.640 8.303 1.00 27.96 A ATOM 769 H THR 226 21.659 76.679 9.248 1.00 0.00 A ATOM 770 CA THR 226 22.433 76.930 7.268 1.00 26.56 A ATOM 771 CB THR 226 23.478 78.382 8.904 1.00 22.566 A ATOM 772 CGI THR 226 23.478 78.382 8.904 1.00 29.78 A 35 ATOM 773 HGI THR 226 23.478 78.382 8.904 1.00 29.78 A ATOM 773 HGI THR 226 22.4301 78.693 9.288 1.00 20.00 A ATOM 775 C THR 226 22.402 78.102 6.807 1.00 25.78 A ATOM 776 O THR 226 22.709 75.740 6.347 1.00 24.98 A ATOM 777 N ALA 227 22.579 74.412 78.48 1.00 20.19 A ATOM 777 CA ALA 227 22.579 74.412 78.48 1.00 23.49 A ATOM 778 H ALA 227 22.579 74.412 78.48 1.00 23.49 A ATOM 778 CA ALA 227 22.579 76.047 1.00 23.49 A ATOM 778 CA ALA 227 22.992 72.077 6.876 1.00 23.86 A ATOM 780 CB ALA 227 22.992 73.101 3.815 1.00 26.01 A ATOM 781 C ALA 227 22.992 73.101 3.815 1.00 26.01 A ATOM 782 O ALA 227 22.992 73.101 3.815 1.00 26.01 A ATOM 783 N LEU 228 20.614 73.503 5.436 1.00 24.83 A ATOM 785 CA LEU 228 19.470 73.499 4.527 1.00 23.49 A ATOM 786 CB LEU 228 19.470 73.499 4.527 1.00 23.49 A ATOM 787 CG LEU 228 19.470 73.499 4.527 1.00 25.07 A ATOM 789 CD LEU 228 19.470 73.499 4.527 1.00 25.07 A ATOM 780 CB ALA 227 22.118 73.301 3.815 1.00 26.01 A ATOM 787 CG LEU 228 19.470 73.499 4.527 1.00 22.51 A ATOM 787 CG LEU 228 19.567 74.603 3.464 1.00 23.30 A ATOM 789 CD2 LEU 228 19.567 74.603 3.464 1.00 22.30 A ATOM 789 CD2 LEU 228 19.567 74.603 3.464 1.00 22.51 A ATOM 790 C LEU 228 19.547 74.603 3.464 1.00 22.50 A ATOM 791 N THR 230 22.81 19.547 74.603 3.464 1.00 22.50 A ATOM 797 N THR 230 22.337 76.313 2.305 1.00 22.51 A ATOM 798 CD2 LEU 228 19.547 74.603 3.464 1.00 22.59 A ATOM 799 CA THR 230 22.337 76.313 2.305 1.00 22.51 A ATOM 790 C LEU 228 19.547 74.603 3.464 1.00 22.55 A ATOM 790 C LEU 228 19.547 74.603 3.464 1.00 22.99 A ATOM 790 C LEU 228 19.547 74.603 3.464 1.00 22.95 A ATOM 790 C LEU 228 19.547 74.603 3.464 1.00 22.95 A ATOM 790 C A THR 230 22.337 76.310										
ATOM										
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ATOM		MOTA		H TH		21.699	76.679		1.00 0.00	A
ATOM		MOTA	770	CA TH					1.00 26.56	A
ATOM		ATOM	771	CB TH	R 226	23.761	77.426	7.879	1.00 28.59	A
ATOM 774 CG2 THR 226 24.622 78.102 6.807 1.00 25.78 A ATOM 775 C THR 226 22.709 75.740 6.347 1.00 24.98 A ATOM 776 O THR 226 22.912 75.922 5.152 1.00 20.19 A ATOM 777 N ALA 227 22.709 74.525 6.889 1.00 25.81 A ATOM 778 H ALA 227 22.570 74.525 6.889 1.00 25.81 A ATOM 778 H ALA 227 22.570 74.525 6.889 1.00 23.49 A ATOM 779 CA ALA 227 22.953 73.357 6.047 1.00 23.49 A ATOM 780 CB ALA 227 22.972 72.077 6.876 1.00 23.49 A ATOM 781 C ALA 227 22.972 72.077 6.876 1.00 23.49 A ATOM 782 C ALA 227 22.953 73.357 6.047 1.00 23.49 A ATOM 782 C ALA 227 22.953 73.351 6.047 1.00 25.42 A ATOM 782 C ALA 227 22.953 73.301 4.999 1.00 25.42 A ATOM 782 C ALA 227 22.120 73.101 3.815 1.00 26.01 A ATOM 783 N LEU 228 20.614 73.658 6.393 1.00 24.83 A ATOM 784 H LEU 228 20.464 73.658 6.393 1.00 24.83 A ATOM 786 CB LEU 228 19.470 73.499 4.527 1.00 25.07 A ATOM 787 CG LEU 228 19.470 73.499 4.527 1.00 25.07 A ATOM 787 CG LEU 228 16.898 73.513 4.450 1.00 32.31 A ATOM 789 CD2 LEU 228 16.898 73.513 4.450 1.00 32.33 A ATOM 789 CD2 LEU 228 16.898 73.513 4.450 1.00 32.31 A ATOM 790 C LEU 228 15.667 73.911 5.256 1.00 31.46 A ATOM 791 C LEU 228 19.547 74.603 3.464 1.00 23.01 A ATOM 792 N GLY 229 19.960 75.803 3.858 1.00 20.11 A ATOM 794 CA GLY 229 20.204 75.955 4.796 1.00 0.00 A ATOM 795 C GLY 229 20.204 75.955 4.796 1.00 0.00 A ATOM 797 N THR 230 22.337 76.313 2.305 1.00 25.52 A ATOM 799 CA THR 230 22.337 76.313 2.305 1.00 25.52 A ATOM 799 CA THR 230 22.337 76.313 2.305 1.00 25.55 A ATOM 799 CA THR 230 22.341 76.627 1.852 1.00 25.55 A ATOM 799 CA THR 230 22.491 76.274 3.271 1.00 0.00 A ATOM 800 CB THR 230 25.794 75.102 1.266 1.00 18.19 A ATOM 801 CG THR 230 25.794 75.102 1.266 1.00 18.19 A ATOM 802 HG1 THR 230 25.794 75.102 1.266 1.00 18.19 A ATOM 803 CG2 THR 230 23.447 74.964 -0.771 1.00 24.80 A ATOM 806 CB ASP 231 22.203 72.630 0.137 1.00 25.95 A ATOM 807 CB ASP 231 22.203 72.307 0.115 0.444 1.00 26.698 A ATOM 808 CB ASP 231 22.207 73.835 1.884 1.00 25.95 A		ATOM	772	OG1 TH	R 226	23.478	78.382	8.904	1.00 29.78	A
ATOM 775 C THR 226 22.709 75.740 6.347 1.00 24.98 A ATOM 776 O THR 226 22.912 75.922 5.152 1.00 20.19 A ATOM 777 N ALA 227 22.709 74.525 6.889 1.00 25.81 A 40 ATOM 778 H ALA 227 22.547 74.412 7.848 1.00 0.00 A ATOM 779 CA ALA 227 22.953 73.357 6.047 1.00 23.49 A ATOM 778 CB ALA 227 22.953 73.357 6.047 1.00 23.49 A ATOM 780 CB ALA 227 22.972 72.077 6.876 1.00 23.49 A ATOM 781 C ALA 227 22.953 73.351 4.999 1.00 25.42 A ATOM 782 O ALA 227 22.1851 73.301 4.999 1.00 26.01 A 45 ATOM 783 N LEU 228 20.614 73.503 5.436 1.00 24.83 A ATOM 784 H LEU 228 20.614 73.503 5.436 1.00 24.83 A ATOM 785 CA LEU 228 19.470 73.499 4.527 1.00 25.07 A ATOM 786 CB LEU 228 19.470 73.499 4.527 1.00 25.07 A ATOM 787 CG LEU 228 18.167 73.656 5.305 1.00 22.51 A ATOM 788 CD1 LEU 228 16.898 73.513 4.450 1.00 34.21 A ATOM 788 CD2 LEU 228 16.898 73.513 4.450 1.00 34.21 A ATOM 789 CD2 LEU 228 15.667 73.911 5.256 1.00 31.46 A ATOM 791 O LEU 228 19.547 74.603 3.464 1.00 32.03 A ATOM 792 N GLY 229 19.960 75.803 3.858 1.00 2.011 A ATOM 794 CA GLY 229 19.960 75.803 3.858 1.00 20.011 A ATOM 795 C GLY 229 20.050 76.890 2.897 1.00 23.03 A ATOM 796 C GLY 229 20.050 76.890 2.897 1.00 23.03 A ATOM 797 N THR 230 22.337 76.313 2.305 1.00 25.57 A ATOM 798 H THR 230 22.337 76.313 2.305 1.00 25.570 A ATOM 799 CA THR 230 22.337 76.313 2.305 1.00 25.570 A ATOM 799 CA THR 230 22.341 76.032 1.393 1.00 25.570 A ATOM 799 CA THR 230 22.337 76.313 2.305 1.00 25.570 A ATOM 799 CA THR 230 22.337 76.313 2.305 1.00 25.570 A ATOM 800 CB THR 230 22.491 76.274 3.271 1.00 0.00 A ATOM 800 CB THR 230 22.491 76.274 3.271 1.00 0.00 A ATOM 800 CB THR 230 22.491 76.274 3.271 1.00 0.00 A ATOM 800 CB THR 230 22.491 76.324 1.393 1.00 25.570 A ATOM 800 CB THR 230 22.491 76.274 3.271 1.00 24.80 A ATOM 800 CB THR 230 22.491 76.324 0.913 1.00 25.570 A ATOM 800 CB THR 230 23.4467 74.964 -0.771 1.00 24.80 A ATOM 807 H ASP 231 22.575 73.825 0.938 1.00 25.10 A ATOM 808 CB ASP 231 22.203 72.630 0.137 1.00 25.88 A ATOM 809 CB ASP 231 22.272 73.835 1.884 1.00 0.00 A	35	ATOM	773	HG1 TH	R 226	24.301	78.693	9.288	1.00 0.00	A
ATOM 775 C THR 226 22.709 75.740 6.347 1.00 24.98 A ATOM 776 O THR 226 22.912 75.922 5.152 1.00 20.19 A ATOM 777 N ALA 227 22.709 74.525 6.889 1.00 25.81 A 40 ATOM 778 H ALA 227 22.547 74.412 7.848 1.00 0.00 A ATOM 779 CA ALA 227 22.953 73.357 6.047 1.00 23.49 A ATOM 778 CB ALA 227 22.953 73.357 6.047 1.00 23.49 A ATOM 780 CB ALA 227 22.972 72.077 6.876 1.00 23.49 A ATOM 781 C ALA 227 22.953 73.351 4.999 1.00 25.42 A ATOM 782 O ALA 227 22.1851 73.301 4.999 1.00 26.01 A 45 ATOM 783 N LEU 228 20.614 73.503 5.436 1.00 24.83 A ATOM 784 H LEU 228 20.614 73.503 5.436 1.00 24.83 A ATOM 785 CA LEU 228 19.470 73.499 4.527 1.00 25.07 A ATOM 786 CB LEU 228 19.470 73.499 4.527 1.00 25.07 A ATOM 787 CG LEU 228 18.167 73.656 5.305 1.00 22.51 A ATOM 788 CD1 LEU 228 16.898 73.513 4.450 1.00 34.21 A ATOM 788 CD2 LEU 228 16.898 73.513 4.450 1.00 34.21 A ATOM 789 CD2 LEU 228 15.667 73.911 5.256 1.00 31.46 A ATOM 791 O LEU 228 19.547 74.603 3.464 1.00 32.03 A ATOM 792 N GLY 229 19.960 75.803 3.858 1.00 2.011 A ATOM 794 CA GLY 229 19.960 75.803 3.858 1.00 20.011 A ATOM 795 C GLY 229 20.050 76.890 2.897 1.00 23.03 A ATOM 796 C GLY 229 20.050 76.890 2.897 1.00 23.03 A ATOM 797 N THR 230 22.337 76.313 2.305 1.00 25.57 A ATOM 798 H THR 230 22.337 76.313 2.305 1.00 25.570 A ATOM 799 CA THR 230 22.337 76.313 2.305 1.00 25.570 A ATOM 799 CA THR 230 22.341 76.032 1.393 1.00 25.570 A ATOM 799 CA THR 230 22.337 76.313 2.305 1.00 25.570 A ATOM 799 CA THR 230 22.337 76.313 2.305 1.00 25.570 A ATOM 800 CB THR 230 22.491 76.274 3.271 1.00 0.00 A ATOM 800 CB THR 230 22.491 76.274 3.271 1.00 0.00 A ATOM 800 CB THR 230 22.491 76.274 3.271 1.00 0.00 A ATOM 800 CB THR 230 22.491 76.324 1.393 1.00 25.570 A ATOM 800 CB THR 230 22.491 76.274 3.271 1.00 24.80 A ATOM 800 CB THR 230 22.491 76.324 0.913 1.00 25.570 A ATOM 800 CB THR 230 23.4467 74.964 -0.771 1.00 24.80 A ATOM 807 H ASP 231 22.575 73.825 0.938 1.00 25.10 A ATOM 808 CB ASP 231 22.203 72.630 0.137 1.00 25.88 A ATOM 809 CB ASP 231 22.272 73.835 1.884 1.00 0.00 A		MOTA	774	CG2 TH	R 226	24.622	78.102	6.807	1.00 25.78	A
ATOM 776 O THR 226 22.912 75.922 5.152 1.00 20.19 A ATOM 777 N ALA 227 22.709 74.525 6.889 1.00 25.81 A ATOM 778 H ALA 227 22.547 74.412 7.848 1.00 0.00 A ATOM 779 CA ALA 227 22.953 73.357 6.047 1.00 23.49 A ATOM 780 CB ALA 227 22.952 73.357 6.047 1.00 23.49 A ATOM 781 C ALA 227 22.972 72.077 6.876 1.00 23.86 A ATOM 782 C ALA 227 22.120 73.301 4.999 1.00 25.42 A ATOM 782 C ALA 227 22.120 73.101 3.815 1.00 26.01 A ATOM 783 N LEU 228 20.614 73.503 5.436 1.00 24.83 A ATOM 784 H LEU 228 20.464 73.658 6.393 1.00 0.00 A ATOM 785 CA LEU 228 19.470 73.499 4.527 1.00 25.07 A ATOM 786 CB LEU 228 18.167 73.656 5.305 1.00 22.517 A ATOM 787 CG LEU 228 16.898 73.513 4.450 1.00 23.33 A ATOM 788 CD1 LEU 228 16.898 73.513 4.450 1.00 34.21 A ATOM 789 CD2 LEU 228 15.667 73.911 5.256 1.00 31.46 A ATOM 790 C LEU 228 15.667 73.911 5.256 1.00 31.46 A ATOM 791 C LEU 228 19.547 74.603 3.464 1.00 23.01 A ATOM 792 N GLY 229 19.560 75.803 3.858 1.00 20.11 A ATOM 793 H GLY 229 20.204 75.955 4.796 1.00 20.01 A ATOM 795 C GLY 229 19.960 75.803 3.858 1.00 20.11 A ATOM 796 C GLY 229 20.204 75.955 4.796 1.00 20.00 A ATOM 798 H THR 230 22.337 76.313 2.305 1.00 25.69 A ATOM 798 H THR 230 22.337 76.313 2.305 1.00 25.89 A ATOM 798 H THR 230 22.337 76.313 2.305 1.00 25.69 A ATOM 799 CA THR 230 22.337 76.313 2.305 1.00 25.570 A ATOM 798 H THR 230 22.337 76.313 2.305 1.00 25.570 A ATOM 800 CB THR 230 22.341 76.022 1.323 1.00 25.52 A ATOM 800 CB THR 230 22.347 76.274 3.271 1.00 0.00 A ATOM 800 CB THR 230 22.347 76.274 3.271 1.00 25.58 A ATOM 801 CG1 THR 230 22.491 76.274 3.271 1.00 25.59 A ATOM 803 CG2 THR 230 23.447 74.964 -0.771 1.00 26.69 A ATOM 804 C THR 230 23.447 74.964 -0.771 1.00 25.69 A ATOM 807 H ASP 231 22.255 73.820 0.938 1.00 25.50 A ATOM 808 CA ASP 231 22.255 73.820 0.938 1.00 25.50 A ATOM 808 CA ASP 231 22.203 72.630 0.137 1.00 22.95 A ATOM 808 CA ASP 231 22.203 72.630 0.137 1.00 24.88 A ATOM 809 CB ASP 231 22.203 70.115 0.444 1.00 26.688 A		ATOM	775	C TH	R 226	22.709	75.740			
## ATOM   777 N   ALA   227   22.709   74.525   6.889   1.00   25.81   A   ATOM   778   H   ALA   227   22.547   74.412   7.848   1.00   0.00   A   ATOM   779   CA   ALA   227   22.953   73.357   6.047   1.00   23.49   A   ATOM   780   CB   ALA   227   22.953   73.357   6.047   1.00   23.46   A   ATOM   781   C   ALA   227   22.972   72.077   6.876   1.00   23.86   A   ATOM   782   O   ALA   227   22.120   73.101   3.815   1.00   25.42   A   ATOM   783   N   LEU   228   20.614   73.503   5.436   1.00   24.83   A   ATOM   784   H   LEU   228   20.614   73.503   5.436   1.00   25.07   A   ATOM   785   CA   LEU   228   20.614   73.658   6.993   1.00   0.00   A   ATOM   786   CB   LEU   228   19.470   73.499   4.527   1.00   25.07   A   ATOM   786   CB   LEU   228   18.167   73.656   5.305   1.00   22.51   A   ATOM   787   CG   LEU   228   16.775   72.087   3.969   1.00   32.33   A   ATOM   788   CD1   LEU   228   16.775   72.087   3.969   1.00   32.33   A   ATOM   780   CD2   LEU   228   15.667   73.911   5.256   1.00   31.46   A   ATOM   790   C   LEU   228   19.219   74.603   3.868   1.00   23.01   A   ATOM   791   O   LEU   228   19.219   74.373   2.300   1.00   26.47   A   ATOM   793   H   GLY   229   20.054   75.955   4.796   1.00   0.01   A   ATOM   794   CA   GLY   229   20.054   75.955   4.796   1.00   0.01   A   ATOM   797   N   THR   230   22.337   76.313   2.305   1.00   23.82   A   ATOM   797   N   THR   230   22.337   76.313   2.305   1.00   25.50   A   ATOM   799   CA   THR   230   22.349   76.726   3.261   1.00   0.50   A   ATOM   800   CB   THR   230   22.337   76.313   2.305   1.00   25.50   A   ATOM   800   CB   THR   230   23.441   76.032   1.393   1.00   25.50   A   ATOM   804   C   THR   230   23.441   76.032   1.393   1.00   25.50   A   ATOM   804   C   THR   230   23.447   76.726   3.261   1.00   0.00   A   ATOM   804   C   THR   230   23.447   75.750   2.182   1.00   25.50   A   ATOM   805   O   THR   230   23.467   74.964   -0.771   1.00   24.80   A   ATOM   805   O   THR   230   23.467										
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## ATOM   783   N   LEU   228   20.614   73.503   5.436   1.00   26.01   A   ATOM   784   H   LEU   228   20.614   73.503   5.436   1.00   24.83   A   ATOM   785   CA   LEU   228   19.470   73.499   4.527   1.00   25.07   A   ATOM   786   CB   LEU   228   19.470   73.499   4.527   1.00   25.07   A   ATOM   787   CG   LEU   228   18.167   73.656   5.305   1.00   22.51   A   ATOM   787   CG   LEU   228   16.898   73.513   4.450   1.00   34.21   A   ATOM   788   CD1   LEU   228   15.667   73.911   5.256   1.00   32.33   A   ATOM   789   CD2   LEU   228   15.667   73.911   5.256   1.00   31.46   A   ATOM   790   C   LEU   228   19.547   74.603   3.464   1.00   23.01   A   ATOM   791   O   LEU   228   19.219   74.373   2.300   1.00   26.47   A   ATOM   792   N   GLY   229   19.960   75.803   3.858   1.00   20.11   A   ATOM   792   N   GLY   229   20.204   75.955   4.796   1.00   0.00   A   ATOM   794   CA   GLY   229   20.204   75.955   4.796   1.00   20.39   A   ATOM   795   C   GLY   229   20.050   76.890   2.897   1.00   22.39   A   ATOM   796   O   GLY   229   20.865   76.706   0.658   1.00   25.69   A   ATOM   797   N   THR   230   22.337   76.313   2.305   1.00   25.88   A   ATOM   797   N   THR   230   22.337   76.313   2.305   1.00   25.50   A   ATOM   799   CA   THR   230   22.491   76.274   3.305   1.00   25.570   A   ATOM   800   CB   THR   230   23.441   76.032   1.393   1.00   25.70   A   ATOM   800   CB   THR   230   23.441   76.032   1.393   1.00   25.754   A   ATOM   801   CG   THR   230   23.148   74.879   0.424   1.00   26.69   A   ATOM   805   O   THR   230   23.148   74.879   0.424   1.00   26.69   A   ATOM   805   O   THR   230   23.148   74.879   0.424   1.00   26.69   A   ATOM   806   N   ASP   231   22.525   73.835   1.884   1.00   0.00   A   ATOM   806   N   ASP   231   22.525   73.835   1.884   1.00   0.00   A   ATOM   806   N   ASP   231   22.527   73.835   1.884   1.00   0.00   A   ATOM   808   CA   ASP   231   22.272   73.835   1.844   1.00   0.00   22.95   A   ATOM   808   CA   ASP   23										
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ATOM 809 CB ASP 231 21.702 71.504 1.050 1.00 14.71 A ATOM 810 CG ASP 231 21.903 70.115 0.444 1.00 26.88 A	70	ATOM	808	CA AS	P 231				1.00 22.95	A
ATOM 810 CG ASP 231 21.903 70.115 0.444 1.00 26.88 A		ATOM	809	CB AS	P 231	21.702	71.504	1.050	1.00 14.71	
		MOTA	810	CG AS	P 231					
		MOTA		OD1 AS			70.004			

			_						
	ATOM	812	OD2 ASP	231	21.722	69.124	1.183	1.00 32.43	A
	MOTA	813	C ASP	231	21.149	72.943	-0.900	1.00 25.92	A
	ATOM	814	O ASP	231	21.167	72.412	-2.019	1.00 22.17	A
_	ATOM	815	N THR	232	20.216	73.803	-0.513	1.00 30.41	A
5	MOTA	816	H THR	232	20.257	74.169	0.395	1.00 0.00	A
	ATOM	817	CA THR	232	19.138	74.216	-1.391	1.00 27.31	A
	ATOM	818	CB THR	232	18.059	74.977	-0.578	1.00 31.03	A
	MOTA	819	OG1 THR	232	17.404	74.051	0.299	1.00 30.78	A
	ATOM	820	HG1 THR	232	16.732	74.513	0.807	1.00 0.00	A
10	ATOM	821	CG2 THR	232	17.023	75.618	-1.497	1.00 22.38	A
	ATOM	822	C THR	232	19.716	75.095	-2.502	1.00 27.81	A
	ATOM	823	O THR	232	19.325	74.978	-3.659	1.00 27.44	A
	ATOM	824	N ALA	233	20.676	75.946	-2.148	1.00 27.86	A
	ATOM	825	H ALA	233	20.957	75.979	-1.210	1.00 0.00	A
15	ATOM	826	CA ALA	233	21.321	76.830	-3.112	1.00 31.80	A
	ATOM	827	CB ALA	233	22.162	77.876	-2.381	1.00 27.63	A
	ATOM	828	C ALA	233	22.195	76.042	-4.095	1.00 35.25	A
	ATOM	829	O ALA	233	22.341	76.431	-5.255	1.00 37.14	A
	ATOM	830	N ALA	234	22.776	74.940	-3.632	1.00 35.16	A
20	ATOM	831	H ALA	234	22.638	74.681	-2.696	1.00 0.00	A
	ATOM	832	CA ALA	234	23.613	74.111	-4.486	1.00 37.73	A
	ATOM	833	CB ALA	234	24.552	73.271	-3.651	1.00 41.51	A
	ATOM	834	C ALA	234	22.712	73.205	-5.293	1.00 40.15	A
	ATOM	835	O ALA	234	23.045	72.806	-6.407	1.00 40.08	A
25	ATOM	836	N LYS	235	21.556	72.897	-4.719	1.00 38.44	A
20	ATOM	837	H LYS	235	21.342	73.275	-3.841	1.00 0.00	A
	ATOM	838	CA LYS	235	20.601	72.013	-5.361	1.00 37.80	A
	ATOM	839	CB LYS	235	19.826	71.223	-4.299	1.00 37.00	A
	ATOM	840	CG LYS	235	20.401	69.856	-3.977	1.00 40.19	A
30	ATOM	841	CD LYS	235	19.542	69.129	-2.957	1.00 40.24	A
50	ATOM	842	CE LYS	235	19.458	67.642	-3.268	1.00 40.24	A
	ATOM	843	NZ LYS	235	18.951	66.862	-2.102	1.00 40.62	Ā
	ATOM	844	HZ1 LYS	235	17.999	67.200	-1.848	1.00 0.00	A
	ATOM	845	HZ2 LYS	235	19.591	66.994	-1.293	1.00 0.00	Ā
35	ATOM	846	HZ3 LYS	235	18.907	65.855	-2.351	1.00 0.00	A
33	ATOM	847	C LYS	235	19.605	72.732	-6.253	1.00 37.03	A
	ATOM	848	O LYS	235	19.199	72.193	-7.282	1.00 37.66	A
	ATOM	849	N GLU	236	19.217	73.947	-5.873	1.00 37.00	A
	ATOM	850	H GLU	236	19.615	74.355	-5.080	1.00 0.00	A
40	ATOM	851	CA GLU	236	18.210	74.677	-6.640	1.00 39.41	A
40	ATOM	852	CB GLU	236	17.025	75.022	-5.736	1.00 39.41	
	ATOM	853	CG GLU	236	16.053	73.022	-5.542	1.00 40.31	A
	ATOM	854	CD GLU	236	15.185	74.050	-3.342 $-4.312$	1.00 47.24	A A
	ATOM	855	OE1 GLU	236	14.414	75.033	-4.259	1.00 50.19	
45	ATOM	856	OE1 GLU	236	15.274	73.203	-3.399	1.00 31.34	A A
43	ATOM	857	C GLU	236	18.650	75.203	-7.361	1.00 49.31	
	ATOM	858	O GLU	236	18.484	76.043	-8.574	1.00 37.37	A A
	ATOM	859	N ALA	237	19.182	76.893	-6.611	1.00 39.16	A
	ATOM	860					-5.646		
50			H ALA	237	19.280	76.749		1.00 0.00	A
50	ATOM	861	CA ALA	237	19.622	78.153	-7.197	1.00 33.79	A
	ATOM	862	CB ALA	237	20.292	79.031	-6.125	1.00 22.28	A
	ATOM	863	C ALA	237	20.586	77.906	-8.357	1.00 31.23	A
	ATOM	864	O ALA	237	20.550	78.610	-9.363	1.00 29.31	A
55	ATOM	865	N PHE	238	21.433	76.889	-8.208	1.00 33.83	A
33	ATOM	866	H PHE	238	21.384	76.354	-7.391	1.00 0.00	A
	MOTA	867	CA PHE	238	22.428	76.545	-9.220	1.00 33.21	A
	ATOM	868	CB PHE	238	23.691	75.985	-8.558	1.00 33.12	A
	ATOM	869	CG PHE	238	24.552	77.026	-7.908	1.00 33.07	A
<b>(0</b>	ATOM	870	CD1 PHE	238	25.030	76.834	-6.616	1.00 32.77	A
60	MOTA	871	CD2 PHE	238	24.882	78.195	-8.580	1.00 29.14	A
	MOTA	872	CE1 PHE	238	25.821	77.792	-5.999	1.00 29.30	A
	ATOM	873	CE2 PHE	238	25.672	79.158	-7.976	1.00 36.10	A
	ATOM	874	CZ PHE	238	26.146	78.957	-6.676	1.00 37.20	A
<i>-</i> -	ATOM	875	C PHE	238	21.934		-10.233	1.00 35.57	A
65	ATOM	876	O PHE	238	22.487		-10.347	1.00 34.78	A
	MOTA	877	N THR	239	20.894		-10.971	1.00 41.07	A
	ATOM	878	H THR	239	20.472		-10.834	1.00 0.00	A
	MOTA	879	CA THR	239	20.370		-11.984	1.00 46.32	A
	MOTA	880	CB THR	239	19.073		-11.508	1.00 46.28	A
70	MOTA	881	OG1 THR	239	18.000		-11.474	1.00 46.22	A
	MOTA	882	HG1 THR	239	17.861		-12.353	1.00 0.00	A
	MOTA	883	CG2 THR	239	19.272		-10.116	1.00 51.02	A
	ATOM	884	C THR	239	20.107	75.780	-13.248	1.00 45.38	A

	ATOM	885	O THR	239	19.735	76.951 -13.185	1.00 46.02	A
	ATOM	886	N GLU		20.320	75.152 -14.396		A
	ATOM	887	H GLU		20.614	74.216 -14.386		A
_	ATOM	888	CA GLU		20.123	75.825 -15.667		A
5	MOTA	889	CB GLU		20.289	74.833 -16.813		A
	MOTA	890	CG GLU		21.543 22.735	73.981 -16.702		A
	ATOM ATOM	891 892	CD GLU OE1 GLU		23.662	74.606 -17.398 75.079 -16.700		A A
	ATOM	893	OE1 GLU		22.741	74.625 -18.645		A
10	ATOM	894	C GLU		18.737	76.427 -15.691		A
10	ATOM	895	O GLU		18.482	77.397 -16.397		A
	ATOM	896	N ALA		17.848	75.844 -14.893		A
	ATOM	897	H ALA		18.132	75.082 -14.346		A
	ATOM	898	CA ALA		16.468	76.299 -14.808		A
15	ATOM	899	CB ALA		15.611	75.237 -14.132		A
	ATOM	900	C ALA	241	16.376	77.600 -14.036	1.00 49.38	A
	MOTA	901	O ALA	241	15.542	78.453 -14.336	1.00 52.67	A
	MOTA	902	N ARG		17.238	77.748 -13.039		A
••	MOTA	903	H ARG		17.889	77.041 -12.853		A
20	MOTA	904	CA ARG		17.226	78.944 -12.221		A
	MOTA	905	CB ARG		17.408	78.562 -10.744		A
	ATOM	906	CG ARG		16.493	77.376 -10.317		A
	MOTA	907	CD ARG		15.817	77.532 -8.931		A
25	ATOM ATOM	908 909	NE ARG HE ARG		14.782 14.958	78.570 -8.877 79.399 -9.365		A A
23	ATOM	910	CZ ARG		13.635	78.491 -8.196		A A
	ATOM	911	NH1 ARG		13.313	77.413 -7.488		A
	ATOM		HH11 ARG		13.952	76.653 -7.416		A
	ATOM		HH12 ARG		12.442	77.383 -6.994		A
30	ATOM	914	NH2 ARG		12.807	79.524 -8.203		A
	ATOM	915	HH21 ARG		13.057	80.361 -8.690		A
	ATOM	916	HH22 ARG	242	11.938	79.475 -7.709	1.00 0.00	A
	ATOM	917	C ARG	242	18.277	79.944 -12.681	1.00 46.22	A
~ =	ATOM	918	O ARG		18.564	80.913 -11.984		A
35	ATOM	919	N GLY		18.850	79.704 -13.860		A
	ATOM	920	H GLY		18.612	78.899 -14.365		A
	ATOM	921	CA GLY		19.832	80.634 -14.398		A
	ATOM	922 923	C GLY		21.289	80.231 -14.535		A
40	ATOM ATOM	924	O GLY N ALA		21.993 21.750	80.797 -15.371 79.276 -13.731		A A
70	ATOM	925	H ALA		21.730	78.857 -13.086		A
	ATOM	926	CA ALA		23.144	78.838 -13.789		A
	ATOM	927	CB ALA		23.315	77.543 -13.015		A
	ATOM	928	C ALA		23.635	78.656 -15.223		A
45	ATOM	929	O ALA	244	22.941	78.070 -16.054		A
	MOTA	930	N ARG	245	24.833	79.159 -15.505	1.00 35.79	A
	ATOM	931	H ARG		25.344	79.603 -14.803		A
	ATOM	932	CA ARG		25.406	79.057 -16.839		A
50	ATOM	933	CB ARG		26.112	80.375 -17.205		A
50	ATOM	934	CG ARG		25.170	81.597 -17.186		A
	MOTA	935	CD ARG		25.919	82.937 -17.270		A
	ATOM ATOM	936 937	NE ARG HE ARG		26.703 26.520	83.246 -16.071 82.731 -15.258		A A
	ATOM	938	CZ ARG		27.636	84.192 -16.014		A
55	ATOM	939	NH1 ARG		27.911	84.933 -17.085		A
	ATOM		HH11 ARG		27.400	84.791 -17.934		A
	ATOM		HH12 ARG		28.616	85.640 -17.039		A
	ATOM	942	NH2 ARG		28.304	84.397 -14.887		A
	ATOM	943	HH21 ARG	245	28.098	83.847 -14.077	1.00 0.00	A
60	MOTA	944	HH22 ARG	245	29.009	85.102 -14.847	1.00 0.00	A
	ATOM	945	C ARG		26.366	77.868 -16.937		A
	ATOM	946	O ARG		27.190	77.640 -16.053		A
	ATOM	947	N ARG		26.243	77.120 -18.030		A
65	ATOM	948	H ARG		25.576	77.378 -18.700		A
65	MOTA	949	CA ARG		27.052	75.931 -18.279		A
	ATOM	950 951	CB ARG		26.710	75.351 -19.655		A
	ATOM	951 952	CG ARG		25.360 25.331	74.674 -19.728		A
	ATOM ATOM	952 953	CD ARG NE ARG		25.331 24.144	73.599 -20.805 72.756 -20.688		A
70	ATOM	953 954	HE ARG		23.939	72.373 -19.811		A A
, 0	ATOM	955	CZ ARG		23.324	72.473 -21.697		A
	ATOM	956	NH1 ARG		22.267	71.694 -21.494		A
	MOTA		HH11 ARG		22.087	71.323 -20.583		A

	ATOM	958	HH12 AF	G 246	21.650	71.482	-22.252	1.00 0.00	A
	MOTA	959	NH2 AF	G 246	23.561	72.966	-22.908	1.00 76.75	A
	ATOM	960	HH21 AF	G 246	24.357	73.550	-23.064	1.00 0.00	A
	MOTA	961	HH22 AF	G 246	22.943	72.750	-23.664	1.00 0.00	A
5	ATOM	962	C AF	G 246	28.557	76.143	-18.200	1.00 37.90	A
	ATOM	963	O AF	G 246	29.149	76.779	-19.074	1.00 41.30	A
	ATOM	964	N GI	Y 247	29.172	75.602	-17.157	1.00 30.93	A
	MOTA	965	H GI	Y 247	28.658	75.119	-16.478	1.00 0.00	A
	ATOM	966	CA GI	Y 247	30.610	75.728	-17.019	1.00 33.39	A
10	ATOM	967	C GI	Y 247	31.104	77.062	-16.515	1.00 34.40	A
	ATOM	968	O GI	Y 247	32.280	77.394	-16.648	1.00 37.30	A
	ATOM	969	N VA	L 248	30.206	77.853	-15.947	1.00 37.33	A
	ATOM	970	H V	L 248	29.266	77.576	-15.906	1.00 0.00	A
	ATOM	971	CA V	L 248	30.617		-15.390	1.00 33.83	A
15	ATOM	972	CB VA	L 248	29.506	80.168	-15.526	1.00 29.27	A
	ATOM	973	CG1 V	L 248	29.660		-14.471	1.00 27.00	A
	ATOM	974	CG2 V	L 248	29.559	80.764	-16.916	1.00 18.63	A
	ATOM	975	C VF	L 248	30.905	78.819	-13.926	1.00 38.78	A
	ATOM	976	O V	L 248			-13.296	1.00 44.51	A
20	ATOM	977	N L		31.985		-13.397	1.00 37.56	A
	ATOM	978	H L		32.536		-13.946	1.00 0.00	A
	MOTA	979	CA LY		32.362		-12.012	1.00 39.22	A
	MOTA	980	CB LY			79.894	-11.660	1.00 42.55	Α
	ATOM	981	CG LY			79.585	-10.262	1.00 49.76	A
25	ATOM	982	CD L7		34.281	78.082	-9.992	1.00 50.58	Α
	ATOM	983	CE LY			77.781	-8.498	1.00 53.51	A
	ATOM	984	NZ L7			77.621	-8.011	1.00 56.75	A
	ATOM	985	HZ1 LY			78.498	-8.188	1.00 0.00	A
20	ATOM	986	HZ2 LY			76.834	-8.518	1.00 0.00	A
30	ATOM	987	HZ3 LY			77.418	-6.992	1.00 0.00	A
	ATOM	988	C I'				-11.045	1.00 37.78	A
	ATOM	989	O F?			80.614	-11.120	1.00 39.09	A
	ATOM	990	N T7		30.934	78.602	-10.140	1.00 34.03	A
35	ATOM	991	H L7			77.750	-10.132	1.00 0.00	A
33	MOTA MOTA	992 993	CA LY			78.833 77.537	-9.161 -8.890	1.00 33.73 1.00 32.39	A A
	ATOM	994	CG II			77.111	-10.006	1.00 32.39	A
	ATOM	995	CD T7			75.659	-10.376	1.00 30.32	A
	ATOM	996	CE L			74.777	-9.831	1.00 33.84	A
40	ATOM	997	NZ LY			74.661	-10.810	1.00 37.02	A
70	ATOM	998	HZ1 LY			74.247	-11.692	1.00 0.00	Ā
	ATOM	999	HZ2 LY			75.607	-11.003	1.00 0.00	A
	ATOM	1000	HZ3 LY			74.054	-10.418	1.00 0.00	A
	ATOM	1001	C L			79.326	-7.864	1.00 32.94	A
45	ATOM	1002	0 F?			78.718	-7.341	1.00 31.11	A
	ATOM	1003	N V			80.441	-7.360	1.00 28.36	A
	ATOM	1004	H V			80.901	-7.843	1.00 0.00	A
	ATOM	1005	CA V			80.987	-6.105	1.00 29.32	A
	ATOM	1006	CB V		31.228	82.296		1.00 33.68	A
50	ATOM	1007	CG1 VA	L 251	31.611	82.882	-4.965	1.00 30.93	A
	ATOM	1008	CG2 VA	L 251	32.478	82.030	-7.137	1.00 35.10	A
	MOTA	1009	C VA	L 251	29.308	81.236	-5.142	1.00 27.80	A
	ATOM	1010	O V	L 251		81.672	-5.534	1.00 23.98	A
	ATOM	1011	N ME			80.955	-3.874	1.00 27.02	A
55	MOTA	1012	H ME			80.618	-3.628	1.00 0.00	A
	ATOM	1013	CA ME			81.134	-2.841	1.00 29.16	A
	MOTA	1014	CB ME			79.779	-2.192	1.00 31.45	A
	MOTA	1015	CG ME			79.497	-1.946	1.00 32.24	A
	MOTA	1016	SD ME			77.877	-1.174	1.00 36.40	A
60	MOTA	1017	CE ME			76.900	-2.663	1.00 27.09	A
	ATOM	1018	C ME			82.114	-1.779	1.00 27.61	Α
	ATOM	1019	O ME			82.067	-1.363	1.00 32.25	A
	ATOM	1020	N V			83.028	-1.376	1.00 27.62	A
65	ATOM	1021	H V			83.065	-1.801	1.00 0.00	A
65	ATOM	1022	CA V			83.981	-0.320	1.00 29.51	A
	ATOM	1023	CB VA			85.459	-0.821	1.00 26.29	A
	MOTA	1024	CG1 VA			86.368	0.305	1.00 28.02	A
	ATOM	1025	CG2 V			85.625	-2.024	1.00 23.28	A
70	MOTA	1026	C V			83.825	0.754	1.00 28.07	A
70	ATOM	1027	O VZ			84.333	0.598	1.00 25.71	A
	ATOM	1028	N II			83.107	1.828	1.00 29.62	A n
	ATOM ATOM	1029 1030	H II CA II			82.721 82.874	$1.881 \\ 2.931$	1.00 0.00 1.00 25.76	A A
	AION	1030	CM II	404 ندر	20.000	04.074	4.331	1.00 20.70	A

	ATOM	1031	CB I	LE 2	254	26.933	81.416	3.476	1 00	26.55	А
	ATOM	1032			254	25.851	81.144	4.512		23.36	A
	ATOM	1033			254	26.764	80.415	2.330		23.69	A
	ATOM	1034			254	28.047	79.781	1.869		23.22	A
5	MOTA	1035			254	27.076	83.879	4.053		23.27	A
	ATOM	1036			254	28.222	84.121	4.418		26.33	A
	ATOM	1037			255	26.000	84.452	4.590		19.71	A
	ATOM	1038			255	25.120	84.171	4.270	1.00	0.00	A
	ATOM	1039			255	26.059	85.474	5.631		18.36	A
10	ATOM	1040			255	25.492	86.818	5.063		19.62	A
10	ATOM	1041	CG1 V		255	25.599	87.923	6.080		17.22	A
	ATOM	1041	CG2 V		255	26.254	87.209	3.790		20.74	A
	ATOM	1042									
	ATOM				255	25.220	84.990	6.812		16.43	A
15		1044			255	24.035	84.701	6.649		19.58	A
15	ATOM	1045			256	25.826	84.875	7.990		15.49	A
	ATOM	1046			256	26.770	85.121	8.082	1.00	0.00	A
	ATOM	1047			256	25.084	84.390	9.142		14.90	A
	MOTA	1048			256	25.113	82.858	9.212		14.75	A
20	ATOM	1049	OG1 T		256	24.240	82.400	10.253		13.11	A
20	MOTA	1050			256	24.525	82.758	11.096	1.00	0.00	A
	MOTA	1051			256	26.526	82.378	9.476		12.09	A
	ATOM	1052			256	25.501	84.938	10.494	1.00	20.05	A
	ATOM	1053			256	26.661	85.291	10.724	1.00	16.01	A
	MOTA	1054			257	24.512	84.930	11.385	1.00	21.65	A
25	ATOM	1055	H A		257	23.664	84.542	11.090	1.00	0.00	A
	ATOM	1056	CA A		257	24.557	85.440	12.757	1.00	24.04	A
	ATOM	1057	CB A		257	23.199	86.096	13.031	1.00	29.68	A
	MOTA	1058	CG A	SP 2	257	23.297	87.308	13.891	1.00	38.27	A
	ATOM	1059	OD1 A	SP 2	257	24.426	87.791	14.137	1.00	52.10	A
30	ATOM	1060	OD2 A	SP 2	257	22.228	87.780	14.321	1.00	36.38	A
	ATOM	1061	C A	SP 2	257	24.831	84.444	13.904	1.00	16.57	A
	ATOM	1062	0 A	SP 2	257	25.087	84.859	15.036	1.00	15.92	A
	ATOM	1063	N G	LY 2	258	24.731	83.150	13.643		12.93	A
	ATOM	1064	H G	LY 2	258	24.516	82.837	12.744	1.00	0.00	A
35	ATOM	1065			258	24.950	82.198	14.721		16.21	A
	ATOM	1066	C G	LY 2	258	25.155	80.786	14.229		21.42	A
	ATOM	1067		LY 2	258	25.226	80.552	13.026		16.78	A
	ATOM	1068			259	25.254	79.845	15.167		21.61	A
	ATOM	1069			259	25.190	80.105	16.110	1.00	0.00	A
40	ATOM	1070			259	25.450	78.442	14.832		22.54	A
	ATOM	1071			259	25.801	77.649	16.093		27.50	A
	ATOM	1072			259	26.886	78.305	16.911		38.06	A
	ATOM	1073			259	27.536	77.361	17.891		39.46	A
	ATOM	1074	OE1 G		259	28.417	76.578	17.468		44.28	A
45	MOTA	1075	_		259	27.167	77.410	19.083		40.01	A
	ATOM	1076			259	24.196	77.875	14.187		19.71	A
	ATOM	1077			259	23.093	78.316	14.468		16.96	A
	ATOM	1078			260	24.357	76.886	13.324		21.81	A
	ATOM	1079			260	25.252	76.526		1.00		A
50	ATOM	1080			260	23.197	76.337	12.649		24.30	A
	ATOM	1081			260	23.585	75.761	11.287	1.00		A
	ATOM	1082			260	24.643	74.827	11.404	1.00		A
	ATOM	1083			260	25.412	75.260	11.780	1.00	0.00	A
	ATOM	1084			260	22.492	75.279	13.456		24.11	A
55	MOTA	1085			260	23.123	74.488	14.150		19.93	A
55	ATOM	1086			261	21.166	75.303	13.384	1.00		
	ATOM	1087			261						A
		1088				20.726	76.006	12.864		0.00	A
	ATOM ATOM	1088			261 261	20.352	74.308	14.062 13.876		35.00	A
60						18.862	74.616			38.14	A
00	ATOM	1090			261	18.263	75.417	14.994	1.00		A
	ATOM	1091	CD2 H		261	17.159	75.203	15.749	1.00		A
	ATOM	1092	ND1 H		261	18.809	76.600	15.444		42.06	A
	ATOM	1093	HD1 H		261	19.620	77.019	15.088	1.00	0.00	A
65	ATOM	1094	CE1 H		261	18.071	77.080	16.425		41.84	A
65	ATOM	1095	NE2 H		261	17.062	76.251	16.631	1.00		A
	ATOM	1096	HE2 H		261	16.358	76.361	17.297		0.00	A
	MOTA	1097			261	20.715	73.032	13.316	1.00		A
	ATOM	1098			261	20.886	71.969	13.915	1.00		A
<b>~</b> ^	ATOM	1099			262	20.857	73.173	11.997	1.00		A
70	MOTA	1100			262	20.705	74.056	11.602	1.00	0.00	A
	ATOM	1101			262	21.224	72.069	11.122	1.00		A
	MOTA	1102			262	20.783	72.372	9.689	1.00		A
	MOTA	1103	CG T	YR 2	262	19.879	71.310	9.137	1.00	62.19	A

	ATOM	1104	CD1	TYR	262	19.511	71.302	7.792	1.00 67.63	A
	MOTA	1105	CE1	TYR	262	18.676	70.297	7.280	1.00 69.78	A
	MOTA	1106	CD2	TYR	262	19.398	70.290	9.960	1.00 66.65	A
_	MOTA	1107	CE2	TYR	262	18.569	69.285	9.465	1.00 69.62	A
5	MOTA	1108	CZ	TYR	262	18.213	69.290	8.125	1.00 71.57	A
	ATOM	1109	OH	TYR	262	17.408	68.282	7.637	1.00 70.23	A
	MOTA	1110	HH	TYR	262	17.185	67.678	8.350	1.00 0.00	A
	ATOM	1111	С	TYR	262	22.728	71.793	11.152	1.00 45.91	A
4.0	ATOM	1112	0	TYR	262	23.270	71.219	10.215	1.00 45.20	A
10	MOTA	1113	N	ASN	263	23.377	72.230	12.233	1.00 47.51	A
	MOTA	1114	H	ASN	263	22.849	72.702	12.906	1.00 0.00	A
	ATOM	1115	CA	ASN	263	24.817	72.066	12.500	1.00 47.67	A
	MOTA	1116	CB	ASN	263	25.022	71.886	14.011	1.00 49.01	A
	ATOM	1117	CG	ASN	263	26.334	72.466	14.504	1.00 54.05	A
15	ATOM	1118	OD1	ASN	263	27.373	71.805	14.449	1.00 54.43	A
	ATOM	1119	ND2	ASN	263	26.290	73.702	15.000	1.00 47.01	A
	MOTA		HD21		263	25.440	74.188	15.032	1.00 0.00	A
	ATOM		HD22	ASN	263	27.130	74.088	15.322	1.00 0.00	A
	MOTA	1122	С	ASN	263	25.434	70.873	11.775	1.00 49.23	A
20	ATOM	1123	0	ASN	263	26.273	71.026	10.881	1.00 46.48	A
	MOTA	1124	N	HIS	264	25.029	69.681	12.197	1.00 48.43	A
	ATOM	1125	H	HIS	264	24.391	69.635	12.939	1.00 0.00	A
	ATOM	1126	CA	HIS	264	25.496	68.439	11.599	1.00 47.59	A
	ATOM	1127	CB	HIS	264	24.755	67.255	12.228	1.00 46.90	A
25	ATOM	1128	CG	HIS	264	23.275	67.462	12.359	1.00 50.04	A
	ATOM	1129	CD2	HIS	264	22.549	68.207	13.229	1.00 53.97	A
	MOTA	1130	ND1	HIS	264	22.360	66.865	11.517	1.00 51.14	A
	MOTA	1131	HD1	HIS	264	22.581	66.256	10.788	1.00 0.00	A
	MOTA	1132	CE1	HIS	264	21.138	67.228	11.864	1.00 53.11	A
30	ATOM	1133	NE2	HIS	264	21.225	68.044	12.898	1.00 55.29	A
	ATOM	1134	HE2	HIS	264	20.471	68.460	13.361	1.00 0.00	A
	MOTA	1135	C	HIS	264	25.132	68.550	10.130	1.00 46.97	A
	MOTA	1136	0	HIS	264	24.666	69.593	9.686	1.00 51.57	A
	ATOM	1137	N	ARG	265	25.348	67.496	9.358	1.00 44.23	A
35	MOTA	1138	H	ARG	265	25.749	66.684	9.732	1.00 0.00	A
	ATOM	1139	CA	ARG	265	24.983	67.554	7.946	1.00 41.47	A
	MOTA	1140	CB	ARG	265	23.473	67.816	7.831	1.00 40.64	A
	ATOM	1141	CG	ARG	265	23.030	68.564	6.591	1.00 43.80	A
	ATOM	1142	CD	ARG	265	21.666	68.091	6.130	1.00 47.91	A
40	ATOM	1143	NE	ARG	265	21.163	68.876	5.005	1.00 56.53	A
	ATOM	1144	HE	ARG	265	21.797	69.449	4.527	1.00 0.00	A
	MOTA	1145	CZ	ARG	265	19.901	68.861	4.588	1.00 58.89	A
	MOTA	1146		ARG	265	19.006	68.099	5.202	1.00 64.72	A
4.7	MOTA		HH11		265	19.281	67.532	5.979	1.00 0.00	A
45	ATOM		HH12		265	18.057	68.088	4.887	1.00 0.00	A
	MOTA	1149		ARG	265	19.530	69.612	3.561	1.00 63.20	A
	ATOM		HH21		265	20.200	70.192	3.097	1.00 0.00	A
	ATOM		HH22		265	18.580	69.600	3.250	1.00 0.00	A
50	ATOM	1152	_	ARG	265	25.777	68.622		1.00 37.16	A
50	ATOM	1153	0	ARG	265	25.768	68.641	5.943	1.00 37.73	A
	MOTA	1154	N	LEU	266	26.466	69.497	7.904	1.00 30.79	A
	ATOM	1155	H	LEU	266	26.433	69.434	8.878	1.00 0.00	A
	ATOM	1156	CA	LEU	266	27.274	70.551	7.290	1.00 37.31	A
55	MOTA	1157 1158	CB	LEU LEU	266	27.832	71.482	8.368	1.00 31.59	A
55	ATOM	1159	CG		266	27.685	73.002	8.258	1.00 31.43	A
	ATOM			LEU	266 266	26.593	73.400	7.273	1.00 36.39	A
	MOTA MOTA	1160	CD2		266	27.383	73.540	9.638	1.00 28.41	A
		1161 1162	C	LEU	266	28.430	69.925	6.523	1.00 42.12	A
60	MOTA MOTA	1162	O	LEU	266	28.719	70.299	5.388	1.00 43.04	A
00	ATOM		N	GLN	267	29.091	68.967	7.164 8.070	1.00 46.26	A
	ATOM	1164 1165	H	GLN	267 267	28.809 30.218	68.723	6.567	1.00 0.00	A
		1166	CA	GLN		30.218	68.269		1.00 48.62	A
	ATOM ATOM	1167	CB CG	GLN GLN	267 267	30.721	67.188 67.601	7.521 8.987	1.00 54.56 1.00 62.75	A
65	ATOM	1168	CD	GLN	267	31.869	67.127	9.787	1.00 62.75	A A
05	ATOM	1169		GLN	267			9.787		A
		1170		GLN	267 267	32.730	66.406 67.527		1.00 71.87	A A
	MOTA MOTA		HE21		267	31.935		11.055	1.00 68.16	A
						31.227	68.098	11.420	1.00 0.00	A
70	MOTA MOTA	1173	HE22		267 267	32.700 29.830	67.231 67.649	11.584 5.231	1.00 0.00	A A
10	ATOM	1173	C O	GLN GLN	267 267	29.830 30.597	67.700		1.00 48.74 1.00 47.96	A
	ATOM	1175	N	LYS	268	28.637	67.067	4.271 5.166	1.00 47.96	A n
	ATOM	1176	H	LYS	268	28.058	67.047	5.955	1.00 45.46	A A
	ATOM	11/0	T,	הידים	200	20.000	0/.04/	2.323	1.00 0.00	A

	ATOM	1177	CA	LYS	268	28.191	66.463	3.924	1.00 45.48	A
	MOTA	1178	CB :	LYS	268	27.048	65.477	4.181	1.00 49.81	A
	ATOM	1179	CG	LYS	268	27.042	64.279	3.240	1.00 56.67	-A
	ATOM	1180	CD	LYS	268	28.157	63.290	3.578	1.00 61.88	A
5	ATOM	1181	CE	LYS	268	29.009	62.946	2.354	1.00 64.81	A
	ATOM	1182		LYS	268	29.927	61.787	2.599	1.00 70.64	A
	MOTA	1183	HZ1		268	29.368	60.945	2.844	1.00 0.00	A
	ATOM	1184	HZ2		268	30.573	62.014	3.383	1.00 0.00	A
10	ATOM	1185	HZ3		268	30.482	61.595	1.740	1.00 0.00	A
10	ATOM	1186		LYS	268	27.744 27.960	67.533	2.939 1.742	1.00 40.50 1.00 40.62	A A
	ATOM ATOM	1187 1188		LYS VAL	268 269	27.133	67.402 68.603	3.434	1.00 40.02	A
	ATOM	1189		VAL	269	26.991	68.684	4.400	1.00 0.00	A
	ATOM	1190		VAL	269	26.676	69.663	2.538	1.00 37.29	A
15	ATOM	1191		VAL	269	25.782	70.685	3.269	1.00 34.20	A
	ATOM	1192	CG1		269	25.492	71.860	2.356	1.00 29.69	A
	MOTA	1193	CG2		269	24.492	70.026	3.703	1.00 31.32	A
	ATOM	1194	C '	VAL	269	27.857	70.404	1.921	1.00 35.64	A
	ATOM	1195	0	VAL	269	27.844	70.725	0.734	1.00 37.28	A
20	MOTA	1196		ILE	270	28.876	70.667	2.731	1.00 31.83	A
	ATOM	1197		ILE	270	28.833	70.374	3.661	1.00 0.00	A
	ATOM	1198		ILE	270	30.052	71.375	2.261	1.00 33.15	A
	ATOM	1199	CB CG2	ILE	270 270	30.971 32.222	71.750 72.469	3.438 2.930	1.00 33.05 1.00 24.49	A A
25	ATOM ATOM	1200 1201	CG2		270	30.209	72.469	4.417	1.00 24.49	A
23	ATOM	1201	CD1		270	30.041	74.059	3.944	1.00 32.31	A
	ATOM	1203		ILE	270	30.835	70.541	1.252	1.00 38.00	A
	ATOM	1204		ILE	270	31.190	71.026	0.176	1.00 34.89	A
	MOTA	1205	N	GLN	271	31.092	69.283	1.603	1.00 37.30	A
30	MOTA	1206		GLN	271	30.776	68.956	2.471	1.00 0.00	А
	MOTA	1207		GLN	271	31.836	68.378	0.735	1.00 40.28	A
	ATOM	1208		GLN	271	32.061	67.038	1.442	1.00 45.96	A
	ATOM ATOM	1209 1210		GLN GLN	271 271	32.724 34.111	65.972 66.365	0.580 0.114	1.00 50.37 1.00 54.51	A A
35	ATOM	1211	OE1		271	34.298	66.806	-1.026	1.00 54.16	A
50	ATOM	1212	NE2		271	35.102	66.201	0.988	1.00 55.62	A
	MOTA	1213	HE21	GLN	271	34.908	65.841	1.879	1.00 0.00	A
	MOTA	1214	HE22	GLN	271	36.004	66.448	0.704	1.00 0.00	A
40	ATOM	1215		GLN	271	31.103	68.154	-0.583	1.00 42.88	A
40	ATOM	1216		GLN	271	31.722	67.846	-1.599	1.00 46.33	A
	ATOM	$\frac{1217}{1218}$		ASP	272 272	29.783 29.330	68.297 68.520	-0.566 0.276	1.00 40.17	A A
	ATOM ATOM	1210		ASP ASP	272	28.999	68.125	-1.778	1.00 41.34	A
	ATOM	1220		ASP	272	27.529	67.885	-1.439	1.00 43.85	A
45	ATOM	1221		ASP	272	27.249	66.451	-1.068	1.00 45.57	A
	ATOM	1222	OD1	ASP	272	27.395	66.103	0.115	1.00 46.69	Α
	ATOM	1223	OD2	ASP	272	26.885	65.663	-1.960	1.00 53.57	A
	ATOM	1224		ASP	272	29.128	69.379	-2.632	1.00 41.62	A
50	ATOM	1225		ASP	272	28.871	69.354		1.00 39.28	A
50	ATOM	1226		CYS	273 273	29.520 29.694	70.477 70.431	-1.992 -1.028	1.00 37.21 1.00 0.00	A A
	ATOM ATOM	1227 1228		CYS CYS	273	29.697	70.431	-2.685	1.00 34.88	A
	ATOM	1229		CYS	273	29.580	72.910	-1.697	1.00 28.59	A
	ATOM	1230		CYS	273	27.871	73.342	-1.278	1.00 31.88	A
55	ATOM	1231		CYS	273	31.078	71.760	-3.326	1.00 34.92	A
	MOTA	1232	0	CYS	273	31.226	72.094	-4.504	1.00 26.50	Α
	MOTA	1233		GLU	274	32.072	71.384	-2.524	1.00 35.57	A
	ATOM	1234		GLU	274	31.847	71.129	-1.606	1.00 0.00	A
60	ATOM	1235		GLU	274 274	33.470	71.329 70.927	-2.924 -1.706	1.00 38.47 1.00 45.16	A A
00	ATOM ATOM	1236 1237		GLU GLU	274	34.305 35.785	70.680	-1.935	1.00 43.10	Ā
	ATOM	1238		GLU	274	36.356	69.705	-0.908	1.00 56.66	A
	ATOM	1239	OE1		274	37.306	70.063	-0.173	1.00 58.10	A
	MOTA	1240	OE2		274	35.846	68.569	-0.833	1.00 62.18	A
65	ATOM	1241	C	GLU	274	33.629	70.318	-4.054	1.00 43.44	A
	MOTA	1242		GLU	274	34.555	70.407	-4.862	1.00 46.62	A
	MOTA	1243		ASP	275	32.713	69.357	-4.112	1.00 44.68	A
	MOTA	1244		ASP	275	32.002	69.326	-3.440	1.00 0.00	A A
70	ATOM ATOM	1245 1246		ASP ASP	275 275	32.757 31.995	68.356 67.104	-5.160 -4.737	1.00 43.67 1.00 48.36	A A
70	ATOM	1246		ASP	275	32.919	65.936	-4.468	1.00 49.82	A
	ATOM	1248	OD1		275	32.936	64.992	-5.286	1.00 54.38	A
	ATOM	1249	OD2		275	33.634	65.969	-3.443	1.00 54.23	A

	MOTA	1250 C	ASP	275	32.158	68.947	-6.428	1.00 43.28	A
	ATOM ATOM	1251 O 1252 N	ASP GLU	275 276	32.578 31.187	68.610 69.840	-7.540 -6.256	1.00 35.41 1.00 39.61	A A
	ATOM	1252 N		276	30.890	70.058	-5.349	1.00 0.00	A
5	MOTA	1254 C		276	30.551	70.503	-7.392	1.00 42.30	A
	ATOM	1255 C		276	29.085	70.815	-7.078	1.00 44.73	A
	ATOM	1256 C		276	28.246	69.581	-6.784	1.00 47.48	A
	ATOM ATOM	1257 CI 1258 OI	D GLU E1 GLU	276 276	26.769 25.950	69.817 69.064	-7.011 -6.437	1.00 50.24 1.00 50.57	A A
10	ATOM		E1 GLU	276	26.428	70.755	-7.762	1.00 30.37	A
	ATOM	1260 C		276	31.314	71.793	-7.678	1.00 40.70	A
	ATOM	1261 0	GLU	276	30.789	72.716	-8.301	1.00 40.89	A
	ATOM	1262 N		277	32.563	71.829	-7.211	1.00 40.17	A
15	ATOM ATOM	1263 H 1264 C		277 277	32.899 33.465	71.045 72.974	-6.732 -7.373	1.00 0.00 1.00 40.38	A A
13	ATOM	1265 CI		277	34.157	72.914	-8.733	1.00 40.38	A
	ATOM	1266 C		277	35.220	71.832	-8.789	1.00 47.84	A
	MOTA		D1 ASN	277	36.408	72.097	-8.578	1.00 49.04	A
20	ATOM		D2 ASN	277	34.791	70.605	-9.066	1.00 46.30	A
20	ATOM	1269 HD:		277 277	33.840 35.466	70.438 69.895	-9.221 -9.104	1.00 0.00 1.00 0.00	A A
	ATOM ATOM	1270 HD.	ASN ASN	277	32.791	74.327	-7.192	1.00 36.39	A
	ATOM	1272 0		277	32.712	75.137	-8.119	1.00 36.27	A
	ATOM	1273 N		278	32.320	74.569	-5.980	1.00 34.58	A
25	ATOM	1274 H		278	32.422	73.890	-5.281	1.00 0.00	A
	ATOM ATOM	1275 CI		278 278	31.652 30.228	75.819 75.549	-5.665 -5.162	1.00 34.26 1.00 30.91	A A
	ATOM		G2 ILE	278	29.646	76.814	-4.530	1.00 30.31	A
	ATOM		G1 ILE	278	29.368	75.058	-6.331	1.00 26.81	A
30	MOTA		D1 ILE	278	27.955	74.622	-5.936	1.00 27.38	A
	ATOM	1280 C		278	32.424	76.617	-4.616	1.00 35.39	A
	ATOM ATOM	1281 O 1282 N		278 279	32.412 33.105	76.275 77.671	-3.431 -5.062	1.00 35.14 1.00 34.70	A A
	ATOM	1283 H		279	33.105	77.872	-6.022	1.00 0.00	A
35	ATOM	1284 C		279	33.869	78.537	-4.166	1.00 33.01	A
	MOTA	1285 CI		279	34.560	79.647	-4.954	1.00 38.07	A
	ATOM ATOM	1286 CC		279 279	35.956 37.019	79.282 80.222	-5.430 -4.886	1.00 46.02 1.00 49.56	A A
	ATOM		E1 GLN	279	36.779	81.422	-4.726	1.00 40.91	A
40	ATOM		E2 GLN	279	38.205	79.680	-4.601	1.00 48.01	A
	ATOM	1290 HE		279	38.352	78.722	-4.749	1.00 0.00	A
	ATOM	1291 HE		279	38.901	80.273	-4.252	1.00 0.00 1.00 30.48	A
	ATOM ATOM	1292 C 1293 O		279 279	32.900 31.861	79.155 79.680	-3.163 -3.543	1.00 30.48	A A
45	ATOM	1294 N		280	33.253	79.098	-1.882	1.00 31.39	A
	ATOM	1295 н		280	34.114	78.698	-1.641	1.00 0.00	A
	ATOM	1296 C		280	32.388	79.622	-0.833	1.00 32.62	A
	ATOM ATOM	1297 C		280 280	31.864 31.447	78.452 77.246	0.013 -0.823	1.00 31.05 1.00 30.23	A A
50	ATOM	1299 C		280	31.031	76.072	0.033	1.00 29.02	A
	ATOM	1300 N		280	32.172	75.403	0.641	1.00 23.82	A
	ATOM	1301 H		280	32.358	75.574	1.588	1.00 0.00	A
	MOTA MOTA	1302 C:	Z ARG H1 ARG	280 280	32.972 32.756	74.567 74.297	-0.008 -1.290	1.00 30.22 1.00 32.10	A A
55	ATOM	1304 HH		280	31.983	74.717	-1.766	1.00 0.00	A
	ATOM	1305 HH		280	33.362	73.669	-1.778	1.00 0.00	A
	MOTA		H2 ARG	280	33.985	73.996	0.627	1.00 33.41	A
	ATOM	1307 HH		280	34.141	74.190	1.595	1.00 0.00	A
60	ATOM ATOM	1308 HH 1309 C		280 280	34.592 33.046	73.369 80.673	0.138 0.070	1.00 0.00 1.00 31.10	A A
00	ATOM	1310 0		280	34.146	80.477	0.598	1.00 29.04	A
	ATOM	1311 N		281	32.354	81.792	0.231	1.00 27.75	A
	ATOM	1312 H		281	31.499	81.890	-0.231	1.00 0.00	A
65	ATOM ATOM	1313 C		281 281	32.824 32.798	82.879 84.199	1.074 0.303	1.00 30.07 1.00 28.77	A A
03	ATOM	1314 C.		281	33.920	84.348	-0.671	1.00 28.77	A
	ATOM		D1 PHE	281	33.774	83.928	-1.988	1.00 37.93	A
	MOTA		D2 PHE	281	35.136	84.893	-0.272	1.00 33.95	A
70	ATOM		E1 PHE	281	34.830	84.047	-2.894	1.00 38.18	A
70	ATOM		E2 PHE	281 281	36.196 36.042	85.014 84.591	-1.174 -2.481	1.00 31.36 1.00 33.33	A A
	MOTA MOTA	1320 C		281 281	36.042 31.857	84.591	$\frac{-2.481}{2.247}$	1.00 33.33	A A
	ATOM	1322 0		281	30.676	83.214	2.045	1.00 33.33	A

	ATOM	1323	N	SER	282	32.337	82.708	3.463	1.00 27.38	A
	MOTA	1324	H	SER	282	33.286	82.493	3.582	1.00 0.00	A
	ATOM	1325	CA	SER	282	31.455	82.765	4.610	1.00 31.18	A
	MOTA	1326	CB	SER	282	31.462	81.425	5.359	1.00 29.23	A
5	MOTA	1327	OG	SER	282	32.690	81.189	6.020	1.00 25.15	A
	MOTA	1328	$^{\mathrm{HG}}$	SER	282	33.402	81.171	5.376	1.00 0.00	A
	MOTA	1329	C	SER	282	31.777	83.919	5.560	1.00 32.76	A
	MOTA	1330	0	SER	282	32.886	84.044	6.079	1.00 37.88	A
	ATOM	1331	N	ILE	283	30.777	84.766	5.766	1.00 33.62	A
10	MOTA	1332	H	ILE	283	29.927	84.603	5.308	1.00 0.00	A
	MOTA	1333	CA	$_{ m ILE}$	283	30.887	85.921	6.634	1.00 30.37	A
	ATOM	1334	CB	ILE	283	30.324	87.183	5.944	1.00 33.69	A
	$\mathbf{M}$ OTA	1335	CG2	ILE	283	30.920	88.435	6.571	1.00 33.06	A
	ATOM	1336	CG1	ILE	283	30.634	87.144	4.448	1.00 28.09	A
15	ATOM	1337	CD1	ILE	283	30.588	88.512	3.781	1.00 33.55	A
	ATOM	1338	С	ILE	283	30.095	85.671	7.911	1.00 30.75	A
	ATOM	1339	0	ILE	283	28.878	85.485	7.869	1.00 30.38	A
	ATOM	1340	N	ALA	284	30.797	85.658	9.038	1.00 25.22	A
20	ATOM	1341	H	ALA	284	31.767	85.785	8.990	1.00 0.00	A
20	ATOM	1342	CA	ALA	284	30.183	85.462	10.344	1.00 25.92	A
	ATOM	1343	CB	ALA	284	31.034	84.480	11.172	1.00 26.80	A
	MOTA	1344	C	ALA	284	30.026	86.790	11.114	1.00 25.45	A
	ATOM	1345	0	ALA	284	31.025	87.437	11.458	1.00 23.52	A
25	MOTA	1346	N	ILE	285	28.780	87.188	11.379	1.00 21.71	A
25	MOTA	1347	H	ILE	285	28.033	86.646	11.052	1.00 0.00	A
	MOTA	1348	CA	ILE	285	28.484	88.404	12.142	1.00 14.56 1.00 20.57	A
	ATOM	1349	CB	ILE	285	27.122 26.861	89.033	11.672 12.360	1.00 20.37	A A
	ATOM	1350 1351	CG2	ILE	285 285	27.157	90.366 89.301	10.171	1.00 15.00	A
30	ATOM	1351	CG1 CD1	ILE	285 285	25.781	89.470	9.533	1.00 15.00	A
30	ATOM ATOM	1353	CDI	ILE	285	28.427	87.958	13.618	1.00 18.61	A
	ATOM	1354	0	ILE	285	27.631	87.083	13.985	1.00 20.11	A
	ATOM	1355	N	LEU	286	29.295	88.521	14.465	1.00 20.11	A
	ATOM	1356	H	LEU	286	29.905	89.212	14.134	1.00 0.00	A
35	ATOM	1357	CA	LEU	286	29.348	88.131	15.884	1.00 17.79	A
33	ATOM	1358	CB	LEU	286	30.798	88.163	16.409	1.00 20.85	A
	ATOM	1359	CG	LEU	286	31.846	87.099	16.069	1.00 23.26	A
	ATOM	1360	CD1		286	32.975	87.139	17.093	1.00 26.78	A
	ATOM	1361	CD2	LEU	286	31.217	85.739	16.067	1.00 25.33	A
40	ATOM	1362	C	LEU	286	28.501	89.056	16.754	1.00 18.17	A
	ATOM	1363	Ō	LEU	286	28.515	88.951	17.983	1.00 20.22	A
	ATOM	1364	N	GLY	287	27.788	89.969	16.099	1.00 22.67	A
	ATOM	1365	H	GLY	287	27.840	89.999	15.120	1.00 0.00	A
	ATOM	1366	CA	GLY	287	26.941	90.925	16.789	1.00 20.22	A
45	ATOM	1367	С	GLY	287	26.080	90.382	17.913	1.00 16.26	A
	ATOM	1368	0	GLY	287	26.381	90.585	19.089	1.00 23.96	A
	MOTA	1369	N	HIS	288	25.000	89.693	17.572	1.00 22.56	A
	MOTA	1370	H	$\mathtt{HIS}$	288	24.798	89.534	16.627	1.00 0.00	A
	MOTA	1371	CA	HIS	288	24.109	89.168	18.608	1.00 20.44	A
50	ATOM	1372	CB	HIS	288	22.990	88.312	17.970	1.00 19.88	A
	ATOM	1373	CG	HIS	288	21.974	87.804	18.950	1.00 23.39	A
	MOTA	1374	CD2	HIS	288	21.917	86.650	19.654	1.00 17.27	A
	ATOM	1375		HIS	288	20.917	88.571	19.385	1.00 15.20	A
	MOTA	1376		HIS	288	20.679	89.455	19.045	1.00 0.00	A
55	MOTA	1377		HIS	288	20.242	87.909	20.310	1.00 15.13	A
	ATOM	1378		HIS	288	20.832	86.739	20.494	1.00 13.24	A
	MOTA	1379		HIS	288	20.535	86.056	21.118	1.00 0.00	A
	MOTA	1380	С	HIS	288	24.850	88.371	19.715	1.00 17.46	A
	ATOM	1381	0	HIS	288	24.579	88.541	20.902	1.00 17.25	A
60	MOTA	1382	N	TYR	289	25.798	87.525	19.334	1.00 18.14	A
	MOTA	1383	H	TYR	289	26.023	87.431	18.384	1.00 0.00	A
	MOTA	1384	CA	TYR	289	26.505	86.737	20.330	1.00 16.63	A
	ATOM	1385	CB	TYR	289	27.405	85.709	19.647	1.00 25.01	A
~~	MOTA	1386	CG	TYR	289	26.727	84.387	19.312	1.00 26.14	A
65	MOTA	1387		TYR	289	25.631	84.330	18.449	1.00 26.68	A
	ATOM	1388		TYR	289	25.073	83.092	18.064	1.00 29.84	A
	ATOM	1389		TYR	289	27.245	83.176	19.792	1.00 29.68	A
	ATOM	1390		TYR	289	26.697	81.941	19.415	1.00 19.88	A
70	ATOM	1391	CZ	TYR	289	25.624	81.904	18.551	1.00 24.45	A
70	ATOM	1392	OH	TYR	289	25.129	80.680	18.154	1.00 29.76	A
	ATOM	1393	HH	TYR	289	24.390	80.813	17.553	1.00 0.00	A
	ATOM	1394	C	TYR	289	27.323	87.613	21.277	1.00 20.22	A
	MOTA	1395	0	TYR	289	27.369	87.356	22.481	1.00 19.02	A

	ATOM	1396	N	ASN	290	27.956	88.655	20.750	1.00 18.81	A
	ATOM	1397	H	ASN	290	27.904	88.835	19.789	1.00 0.00	A
	ATOM	1398	CA	ASN	290	28.739	89.532	21.621	1.00 15.76	A
	ATOM	1399	CB	ASN	290	29.625	90.469	20.804	1.00 19.19	A
5	ATOM	1400	CG	ASN	290	30.840	89.780	20.231	1.00 22.46	A
-	ATOM	1401		ASN	290	31.270	88.736	20.715	1.00 23.52	A
	ATOM	1402		ASN	290	31.400	90.370	19.186	1.00 25.92	A
	ATOM		HD21		290	31.020	91.202	18.832	1.00 0.00	A
	ATOM		HD22		290	32.188	89.942	18.796	1.00 0.00	A
10	ATOM	1405	C	ASN	290	27.822	90.378	22.493	1.00 15.64	A
10	ATOM	1406	Ö	ASN	290	28.108	90.600	23.672	1.00 23.61	A
	ATOM	1407	N	ARG	291	26.723	90.865	21.924	1.00 15.28	A
	ATOM	1408	H	ARG	291	26.524	90.672	20.984	1.00 0.00	A
	ATOM	1409	CA	ARG	291	25.812	91.687	22.713	1.00 14.06	A
15	ATOM	1410	CB	ARG	291	24.679	92.252	21.845	1.00 14.00	A
13	ATOM	1411	CG	ARG	291	25.183	93.144	20.702	1.00 24.29	A
	ATOM	1411	CD	ARG	291	24.091	94.025	20.702	1.00 24.25	A
	ATOM	1413	NE	ARG	291	23.283	93.333	19.077	1.00 25.20	A
	ATOM	1414	HE	ARG	291	22.365	93.092	19.317	1.00 19.39	A
20		1415	CZ	ARG	291	23.709	93.092	17.859	1.00 34.23	A
20	ATOM	1416		ARG	291	24.948	93.323	17.484	1.00 34.25	A
	ATOM ATOM	1417	HH11		291	25.559	93.796	18.117	1.00 34.43	A
		1417	HH12		291	25.268	93.798	16.568	1.00 0.00	A
	MOTA	1419		ARG	291	22.898	92.381	17.014	1.00 30.49	A
25	ATOM		HH21		291	21.967	92.361	17.014	1.00 30.49	
23	MOTA	1420						16.099		A A
	ATOM				291	23.222 25.268	92.139			
	ATOM	1422	C	ARG	291		90.835	23.845		A
	ATOM	1423	O	ARG	291	25.073	91.317 89.551	24.963 23.576	1.00 17.10 1.00 13.55	A
30	MOTA	1424	N	GLY	292 292	25.073 25.286				A A
30	ATOM	1425	H	GLY	292	24.534	89.193 88.675	22.690 24.616	1.00 0.00 1.00 11.54	
	MOTA	1426	CA	GLY				25.562	1.00 11.54	A A
	MOTA	1427 1428	C	GLY	292 292	25.542 25.169	88.057 87.246	26.411	1.00 22.48	A
	ATOM	1429	O N	GLY ASN	293	26.813	88.425	25.422	1.00 30.00	A
35	MOTA				293	27.049		24.719	1.00 25.61	A
33	MOTA	1430	H	ASN			89.065 87.897	26.281	1.00 0.00	A
	ATOM	1431	CA	ASN	293	27.867 27.567	88.238	27.750	1.00 23.00	A
	ATOM	1432	CB	ASN	293 293	27.587	89.741	28.058	1.00 33.48	A
	ATOM	1433 1434	CG OD1	ASN ASN	293	27.506	90.595	27.185	1.00 41.34	A
40	ATOM	1434		ASN	293	27.988	90.060	29.319	1.00 40.94	A
40	ATOM		HD21		293	28.120	89.353	29.319	1.00 40.94	A
	ATOM ATOM	1437	HD21		293	28.069	91.011	29.537	1.00 0.00	A
		1437	C	ASN	293	28.042	86.369	26.116	1.00 31.86	A
	ATOM ATOM	1439	0	ASN	293	28.265	85.652	27.093	1.00 31.80	A
45	ATOM	1440	N	LEU	294	27.952	85.884	24.877	1.00 25.45	A
43	MOTA	1441	H	LEU	294	27.777	86.501	24.138	1.00 0.00	A
	ATOM	1442	CA	LEU	294	28.102	84.456	24.138	1.00 33.84	A
	ATOM	1443	CB	LEU	294	26.918	83.942	23.747	1.00 33.04	A
	ATOM	1444	CG	LEU	294	25.482	84.323	24.145	1.00 35.78	Ā
50	ATOM	1445		LEU	294	24.601	84.404	22.911	1.00 35.76	A
50	ATOM	1446		LEU	294	24.923	83.299	25.121	1.00 33.54	A
	ATOM	1447	C	LEU	294	29.415	84.154	23.852	1.00 37.21	A
	ATOM	1448	Õ	LEU	294	29.957	85.002	23.137	1.00 37.21	A
	ATOM	1449	N	SER	295	29.930	82.943	24.056	1.00 38.58	A
55	ATOM	1450	H	SER	295	29.465	82.328	24.659	1.00 0.00	A
55	ATOM	1451	CA	SER	295	31.163	82.499	23.409	1.00 38.66	A
	ATOM	1452	CB	SER	295	31.590	81.113	23.930	1.00 40.11	A
	ATOM	1453	OG	SER	295	31.942	81.141	25.306	1.00 45.34	A
	ATOM	1454	HG	SER	295	31.187	81.434	25.822	1.00 0.00	A
60	ATOM	1455	C	SER	295	30.881	82.404	21.914	1.00 33.43	A
00	ATOM	1456	Õ	SER	295	29.780	82.064	21.499	1.00 25.91	A
	ATOM	1457	N	THR	296	31.881	82.703	21.107	1.00 34.10	A
	ATOM	1458	Н	THR	296	32.745	82.966	21.488	1.00 0.00	A
	ATOM	1459	CA	THR	296	31.722	82.649	19.670	1.00 32.52	A
65	ATOM	1460	CB	THR	296	31.966	84.030	19.052	1.00 30.78	A
	ATOM	1461		THR	296	33.072	84.647	19.717	1.00 36.83	A
	ATOM	1462		THR	296	33.856	84.103	19.610	1.00 0.00	A
	ATOM	1463		THR	296	30.740	84.916	19.220	1.00 29.89	A
	ATOM	1464	C	THR	296	32.759	81.673	19.155	1.00 23.03	A
70	ATOM	1465	0	THR	296	32.898	81.483	17.952	1.00 31.90	A
, ,	ATOM	1466	IN	GLU	297	33.482	81.059	20.089	1.00 33.84	A
	ATOM	1467	H	GLU	297	33.304	81.261	21.032	1.00 0.00	A
	ATOM	1468	CA	GLU	297	34.531	80.096	19.763	1.00 39.29	A
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	3 most	1460	CD	207	25 065	70 416	21 026	1 00 45 40	7
,	MOTA	1469 1470	CB GLU CG GLU	297 297	35.065 34.108	79.416 79.377	21.036 22.233	1.00 45.48 1.00 56.35	A A
	ATOM ATOM	1471	CD GLU	297	32.848	78.554	21.977	1.00 58.88	A
	ATOM	1472	OE1 GLU	297	32.842	77.338	22.267	1.00 60.54	A
5	ATOM	1473	OE2 GLU	297	31.855	79.130	21.489	1.00 62.33	A
	MOTA	1474	C GLU	297	34.086	79.024	18.772	1.00 35.45	A
	MOTA	1475	O GLU	297	34.729	78.809	17.748	1.00 34.80	A
	MOTA	1476	N LYS	298	32.982	78.356	19.074	1.00 34.37	A
10	ATOM	1477	H LYS	298	32.498	78.581	19.895	1.00 0.00	A
10	MOTA	1478	CA LYS	298 298	32.466 31.520	77.300 76.414	18.213 19.007	1.00 35.58 1.00 31.26	A A
	ATOM ATOM	1479 1480	CB LYS CG LYS	298	32.038	75.026	19.221	1.00 31.20	A
	ATOM	1481	CD LYS	298	30.941	74.125	19.729	1.00 42.14	A
	ATOM	1482	CE LYS	298	31.135	73.832	21.200	1.00 46.89	A
15	MOTA	1483	NZ LYS	298	32.466	74.301	21.688	1.00 50.64	A
	MOTA	1484	HZ1 LYS	298	32.544	75.328	21.550	1.00 0.00	A
	MOTA	1485	HZ2 LYS	298	33.219	73.820	21.158	1.00 0.00	A
	ATOM	1486	HZ3 LYS	298	32.559	74.079	22.701	1.00 0.00	A
20	MOTA MOTA	1487 1488	C LYS O LYS	298 298	31.743 31.765	77.850 77.236	16.992 15.922	1.00 31.74 1.00 32.24	A A
20	ATOM	1489	N PHE	299	31.703	79.005	17.170	1.00 32.24	A
	ATOM	1490	H PHE	299	31.131	79.425	18.053	1.00 0.00	A
	ATOM	1491	CA PHE	299	30.353	79.673	16.102	1.00 28.31	A
	MOTA	1492	CB PHE	299	29.612	80.883	16.703	1.00 27.71	A
25	MOTA	1493	CG PHE	299	29.131	81.904	15.699	1.00 19.45	A
	ATOM	1494	CD1 PHE	299	28.503	81.526	14.516	1.00 15.16	A
	ATOM ATOM	1495 1496	CD2 PHE CE1 PHE	299 299	29.287 28.046	83.261 82.496	15.964 13.616	1.00 16.16 1.00 15.54	A A
	ATOM	1497	CE2 PHE	299	28.832	84.227	15.015	1.00 13.34	A
30	ATOM	1498	CZ PHE	299	28.215	83.851	13.903	1.00 7.56	A
	ATOM	1499	C PHE	299	31.296	80.076	14.966	1.00 27.62	A
	MOTA	1500	O PHE	299	30.999	79.828	13.803	1.00 23.92	A
	MOTA	1501	N VAL	300	32.440	80.667	15.300	1.00 32.50	A
35	ATOM	1502	H VAL	300	32.635 33.419	80.834 81.074	16.246 14.280	1.00 0.00 1.00 40.70	A A
33	ATOM ATOM	1503 1504	CA VAL CB VAL	300 300	34.545	81.950	14.280	1.00 45.83	A
	MOTA	1505	CG1 VAL	300	35.734	81.084	15.280	1.00 49.69	A
	ATOM	1506	CG2 VAL	300	34.988	82.975	13.860	1.00 49.35	A
	MOTA	1507	C VAL	300	34.082	79.887	13.575	1.00 39.59	A
40	MOTA	1508	O VAL	300	34.426	79.974	12.399	1.00 39.52	A
	ATOM	1509	N GLU	301	34.274	78.791 78.787	14.302 15.244	1.00 38.31 1.00 0.00	A
	ATOM ATOM	1510 1511	H GLU CA GLU	301 301	34.001 34.879	77.597	13.736	1.00 39.63	A A
	ATOM	1512	CB GLU	301	35.240	76.607	14.849	1.00 49.28	A
45	ATOM	1513	CG GLU	301	36.060	75.406	14.388	1.00 51.49	A
	ATOM	1514	CD GLU	301	35.928	74.221	15.328	1.00 57.74	A
	MOTA	1515	OE1 GLU	301	34.879	73.542	15.283	1.00 60.72	A
	MOTA	1516	OE2 GLU C GLU	301	36.867 33.933	73.968 76.932	16.114 $12.742$	1.00 58.47 1.00 37.25	A A
50	ATOM ATOM	1517 1518	C GLU O GLU	301 301	34.360	76.469	11.695	1.00 37.23	A
50	ATOM	1519	N GLU	302	32.647	76.880	13.061	1.00 29.99	Ā
	ATOM	1520	H GLU	302	32.332	77.260	13.909	1.00 0.00	A
	MOTA	1521	CA GLU	302	31.713	76.254	12.144	1.00 29.62	A
	ATOM	1522	CB GLU	302	30.345	76.072	12.800	1.00 29.29	A
55	ATOM	1523	CG GLU	302	29.188	76.118 76.218	11.813 12.489	1.00 30.24 1.00 26.05	A
	ATOM ATOM	1524 1525	CD GLU OE1 GLU	302 302	27.839 27.674	75.643	13.581	1.00 24.89	A A
	ATOM	1526	OE2 GLU	302	26.940	76.870	11.925	1.00 30.75	A
	ATOM	1527	C GLU	302	31.574	77.093	10.874	1.00 32.99	A
60	MOTA	1528	O GLU	302	31.445	76.549	9.775	1.00 30.91	A
	MOTA	1529	N ILE	303	31.615	78.416	11.014	1.00 31.38	A
	ATOM	1530	H ILE	303	31.732	78.810	11.904	1.00 0.00	A
	ATOM ATOM	1531 1532	CA ILE CB ILE	303 303	31.486 31.187	79.283 80.752	$9.842 \\ 10.241$	1.00 31.29 1.00 28.58	A A
65	ATOM	1532	CG2 ILE	303	30.822	81.554	9.009	1.00 23.48	A
0.5	ATOM	1534	CG1 ILE	303	30.043	80.800	11.264	1.00 26.97	A
	ATOM	1535	CD1 ILE	303	28.805	80.026	10.852	1.00 24.95	A
	MOTA	1536	C ILE	303	32.773	79.228	9.029	1.00 33.05	A
<b>77.0</b>	MOTA	1537	O ILE	303	32.744	79.181	7.796	1.00 35.02	A
70	ATOM	1538	N LYS	304	33.903	79.248	9.724	1.00 30.79	A A
	ATOM ATOM	1539 1540	H LYS CA LYS	304 304	33.869 35.190	79.332 79.150	10.698 9.060	1.00 0.00 1.00 30.72	A A
	ATOM	1541	CB LYS	304	36.298	78.979	10.118	1.00 30.72	A
					_				

	ATOM	1542	CG LYS	304	37.724	79.320	9.642	1.00 41.97	A
	ATOM	1543	CD LYS	304	38.511	80.155	10.667	1.00 41.17	A
	MOTA	1544	CE LYS	304	39.416	81.173	9.976	1.00 42.05	A
_	ATOM	1545	NZ LYS	304	40.815	80.691 79.820	9.824 9.256	1.00 41.08 1.00 0.00	A A
5	ATOM ATOM	1546 1547	HZ1 LYS HZ2 LYS	304 304	40.823 41.217	80.495	10.764	1.00 0.00	A
	ATOM	1548	HZ3 LYS	304	41.384	81.421	9.350	1.00 0.00	A
	ATOM	1549	C LYS	304	35.100	77.904	8.161	1.00 25.59	A
	ATOM	1550	O LYS	304	35.395	77.951	6.969	1.00 33.47	A
10	MOTA	1551	N SER	305	34.661	76.800	8.767	1.00 26.69	A
	MOTA	1552	H SER	305	34.433	76.870	9.716	1.00 0.00	A
	ATOM	1553	CA SER	305	34.498	75.489	8.125	1.00 22.76	A
	ATOM	1554	CB SER	305	33.932	74.498 74.298	9.144 8.939	1.00 27.40 1.00 24.13	A A
15	ATOM ATOM	1555 1556	OG SER HG SER	305 305	32.539 32.075	75.133	9.030	1.00 24.13	A
13	ATOM	1557	C SER	305	33.635	75.403	6.860	1.00 24.66	A
	ATOM	1558	O SER	305	33.536	74.340	6.239	1.00 27.99	A
	MOTA	1559	N ILE	306	32.983	76.490	6.482	1.00 25.24	A
	MOTA	1560	H ILE	306	33.058	77.317	7.005	1.00 0.00	A
20	MOTA	1561	CA ILE	306	32.154	76.453	5.294	1.00 20.72	A
	MOTA	1562	CB ILE	306	30.828	77.211	5.513	1.00 17.86	A
	MOTA	1563 1564	CG2 ILE	306 306	30.078 29.952	77.326 76.448	4.209 6.510	1.00 20.63 1.00 20.49	A A
	ATOM ATOM	1565	CD1 ILE	306	29.382	77.307	7.603	1.00 19.14	A
25	MOTA	1566	C ILE	306	32.908	77.098	4.156	1.00 16.50	A
	ATOM	1567	O ILE	306	32.689	76.783	2.994	1.00 19.41	A
	MOTA	1568	N ALA	307	33.833	77.979	4.499	1.00 22.89	A
	ATOM	1569	H ALA	307	34.019	78.150	5.446	1.00 0.00	A
20	ATOM	1570	CA ALA	307	34.576	78.686	3.480	1.00 24.83	A
30	ATOM ATOM	1571 1572	CB ALA C ALA	307 307	35.383 35.476	79.794 77.766	4.123 2.665	1.00 30.01 1.00 23.99	A A
	ATOM	1572	C ALA O ALA	307	36.047	76.812	3.187	1.00 21.83	A
	ATOM	1574	N SER	308	35.568	78.035	1.368	1.00 23.95	A
	ATOM	1575	H SER	308	35.037	78.765	0.987	1.00 0.00	A
35	ATOM	1576	CA SER	308	36.445	77.252	0.511	1.00 29.22	A
	ATOM	1577	CB SER	308	36.343	77.740	-0.937	1.00 21.79	A
	MOTA	1578	OG SER	308	35.241	77.1 <b>4</b> 5 77.376	-1.606 -1.149	1.00 28.41 1.00 0.00	A A
	ATOM	1579 1580	HG SER C SER	308 308	34.430 37.870	77.489	1.035	1.00 34.88	A
40	ATOM ATOM	1581	O SER	308	38.119	78.483	1.724	1.00 32.75	A
.0	ATOM	1582	N GLU	309	38.795	76.581	0.722	1.00 40.30	A
	MOTA	1583	H GLU	309	38.537	75.801	0.188	1.00 0.00	A
	MOTA	1584	CA GLU	309	40.191	76.729	1.160	1.00 42.81	A
4~	MOTA	1585	CB GLU	309	40.931	75.385	1.086	1.00 46.85	A
45	ATOM	1586	CG GLU	309	40.454 41.310	74.318 74.231	2.062 3.318	1.00 53.06 1.00 57.34	A A
	ATOM ATOM	1587 1588	CD GLU OE1 GLU	309 309	42.553	74.231	3.215	1.00 57.54	A
	ATOM	1589	OE2 GLU	309	40.734	74.085	4.416	1.00 61.40	A
	ATOM	1590	C GLU	309	40.861	77.715	0.205	1.00 43.24	A
50	MOTA	1591	O GLU	309	40.550	77.718	-0.987	1.00 44.53	A
	MOTA	1592	N PRO	310	41.762	78.581	0.706	1.00 40.58	A
	ATOM	1593	CD PRO	310	42.414	79.532 78.757	-0.216 $2.080$	1.00 41.03 1.00 41.16	A A
	ATOM ATOM	1594 1595	CA PRO CB PRO	310 310	42.250 43.538	79.545	1.899	1.00 41.10	A
55	ATOM	1596	CG PRO	310	43.269	80.379	0.695	1.00 42.72	A
33	ATOM	1597	C PRO	310	41.242	79.519	2.942	1.00 41.57	A
	MOTA	1598	O PRO	310	40.758	80.582	2.553	1.00 35.45	A
	MOTA	1599	N THR	311	40.953	78.976	4.118	1.00 40.54	A
<b>60</b>	MOTA	1600	H THR	311	41.400	78.144	4.378	1.00 0.00	A
60	MOTA	1601	CA THR	311	39.991	79.574	5.033 6.311	1.00 40.87 1.00 39.66	A A
	ATOM ATOM	1602 1603	CB THR OG1 THR	311 311	39.893 39.391	78.738 79.549	7.377	1.00 39.00	A
	ATOM	1603	HG1 THR	311	38.520	79.880	7.146	1.00 0.00	A
	ATOM	1605	CG2 THR	311	41.258	78.200	6.690	1.00 43.68	A
65	ATOM	1606	C THR	311	40.246	81.037	5.413	1.00 44.47	A
	MOTA	1607	O THR	311	39.299	81.802	5.620	1.00 45.91	A
	MOTA	1608	N GLU	312	41.514	81.432	5.510	1.00 45.09	A
	ATOM	1609	H GLU	312	42.234	80.792	5.337	1.00 0.00	A
70	ATOM	1610	CA GLU	312 312	41.839 43.327	82.809 82.954	5.871 6.228	1.00 42.55 1.00 42.74	A A
70	ATOM ATOM	1611 1612	CB GLU CG GLU	312	44.235	81.829	5.726	1.00 42.74	A
	ATOM	1613	CD GLU	312	44.520	80.800	6.799	1.00 41.47	A
	ATOM	1614	OE1 GLU	312	45.706	80.520	7.057	1.00 42.55	A

	ATOM	1615	OE2	GLU	312	43.559	80.274	7.394	1.00 47.20	A
	MOTA	1616	C	GLU	312	41.502	83.747	4.724	1.00 41.45	A
	ATOM	1617	Ō	GLU	312	41.404	84.963	4.901	1.00 41.26	A
	MOTA	1618	N	LYS	313	41.317	83.181	3.542	1.00 37.88	A
5	MOTA	1619	H	LYS	313	41.394	82.207	3.451	1.00 0.00	A
	ATOM	1620	CA	LYS	313	40.997	83.993	2.380	1.00 36.21	A
	ATOM	1621	CB	LYS	313	41.564	83.358	1.116	1.00 33.23	A
	MOTA	1622		LYS	313	41.563	84.300	-0.079	1.00 34.65	A
1.0	MOTA	1623		LYS	313	41.058	83.617	-1.335	1.00 27.45	A
1 <b>0</b>	MOTA	1624		LYS	313	39.861	84.348	-1.905	1.00 29.91	A
	MOTA	1625		LYS	313	39.913	84.435	-3.387	1.00 32.98	A
	MOTA	1626	HZ1		313	39.928	83.476	-3.790 -3.674	1.00 0.00 1.00 0.00	A A
	ATOM	1627	HZ2 HZ3		313 313	40.770 39.073	84.946 84.941	-3.733	1.00 0.00	A A
15	MOTA MOTA	1628 1629	nдз С	LYS	313	39.515	84.249	2.159	1.00 37.37	A
13	ATOM	1630		LYS	313	39.132	85.357	1.789	1.00 40.91	A
	ATOM	1631		HIS	314	38.683	83.234	2.385	1.00 32.67	A
	ATOM	1632	H	HIS	314	39.036	82.382	2.718	1.00 0.00	A
	ATOM	1633	CA	HIS	314	37.250	83.372	2.143	1.00 34.37	A
20	ATOM	1634	CB	HIS	314	36.725	82.171	1.343	1.00 33.80	A
	ATOM	1635	CG	HIS	314	37.658	81.682	0.280	1.00 29.70	A
	ATOM	1636	CD2	HIS	314	38.910	81.168	0.360	1.00 31.43	A
	MOTA	1637	ND1		314	37.307	81.631	-1.051	1.00 29.34	A
	MOTA	1638	HD1		314	36.455	81.936	-1.435	1.00 0.00	A
25	MOTA	1639	CE1		314	38.295	81.109	-1.747	1.00 29.33	A
	ATOM	1640	NE2		314	39.283	80.818	-0.914	1.00 29.14	A
	MOTA	1641	HE2		314	40.137	80.421	-1.175 3.372	1.00 0.00 1.00 35.91	A A
	ATOM ATOM	1642 1643	C O	HIS HIS	314 314	36.368 35.184	83.552 83.860	3.239	1.00 33.91	A
30	ATOM	1644	N	PHE	315	36.920	83.340	4.559	1.00 36.72	A
50	ATOM	1645	H	PHE	315	37.858	83.065	4.622	1.00 0.00	A
	ATOM	1646	CA	PHE	315	36.132	83.512	5.770	1.00 37.19	A
	ATOM	1647	CB	PHE	315	36.552	82.493	6.834	1.00 34.33	A
	ATOM	1648	CG	PHE	315	36.038	82.804	8.214	1.00 26.72	A
35	MOTA	1649	CD1	PHE	315	34.684	82.672	8.519	1.00 30.96	A
	MOTA	1650	CD2		315	36.911	83.225	9.213	1.00 25.93	A
	MOTA	1651	CE1		315	34.209	82.955	9.800	1.00 23.91	A
	MOTA	1652	CE2		315	36.451	83.510	10.494	1.00 28.16	A
40	ATOM	1653	CZ	PHE	315	35.094	83.375 84.928	10.788 6.299	1.00 29.32 1.00 38.47	A A
40	ATOM	1654 1655	С 0	PHE PHE	315 315	36.326 37.449	85.428	6.344	1.00 38.47	A
	MOTA ATOM	1656	N	PHE	316	35.219	85.561	6.685	1.00 41.30	A
	ATOM	1657	H	PHE	316	34.364	85.091	6.602	1.00 0.00	A
	ATOM	1658	CA	PHE	316	35.213	86.918	7.223	1.00 32.16	A
45	ATOM	1659	СВ	PHE	316	34.390	87.856	6.334	1.00 31.62	A
	MOTA	1660	CG	PHE	316	35.057	88.194	5.041	1.00 37.01	A
	MOTA	1661	CD1	PHE	316	34.804	87.437	3.898	1.00 29.79	A
	MOTA	1662		PHE	316	35.979	89.233	4.971	1.00 33.37	A
<b>50</b>	MOTA	1663	CE1		316	35.462	87.705	2.713	1.00 33.51	A
50	ATOM	1664	CE2		316	36.644	89.511	3.786	1.00 37.63 1.00 37.22	A
	ATOM	1665 1666	CZ	PHE PHE	316 316	36.388 34.577	88.745 86.895	2.653 8.596	1.00 37.22	A A
	ATOM ATOM	1667	С 0	PHE	316	33.446	86.467	8.751	1.00 28.70	A
	ATOM	1668	N	ASN	317	35.311	87.355	9.591	1.00 30.17	A
55	ATOM	1669	H	ASN	317	36.220	87.668	9.414	1.00 0.00	A
	ATOM	1670	CA	ASN	317	34.795	87.405	10.939	1.00 31.72	A
	MOTA	1671	CB	ASN	317	35.855	86.917	11.927	1.00 29.33	A
	MOTA	1672	CG	ASN	317	35.485	87.205	13.376	1.00 34.11	A
	MOTA	1673		ASN	317	34.771	88.163	13.667	1.00 38.43	A
60	MOTA	1674		ASN	317	35.983	86.375	14.289	1.00 32.35	A
	MOTA		HD21		317	36.553	85.627	14.018	1.00 0.00	A
	MOTA		HD22		317	35.752	86.550	15.226	1.00 0.00	A
	MOTA	1677	C	ASN	317 317	34.442	88.861 89.686	11.197 $11.440$	1.00 33.41 1.00 35.10	A A
65	MOTA	1678 1679	O N	ASN	317	35.325 33.152	89.175	11.128	1.00 33.10	A
05	ATOM ATOM	1680	N H	VAL VAL	318	32.498	88.478	10.922	1.00 34.27	A
	ATOM	1681	CA	VAL	318	32.689	90.543	11.355	1.00 32.08	Ā
	ATOM	1682	CB	VAL	318	31.629	90.958	10.301	1.00 36.04	A
	ATOM	1683		VAL	318	31.316	92.441	10.426	1.00 35.17	A
70	ATOM	1684		VAL	318	32.147	90.660	8.905	1.00 37.95	A
-	MOTA	1685	C	VAL	318	32.123	90.743	12.762	1.00 25.89	A
	MOTA	1686	0	VAL	318	31.293	89.978	13.238	1.00 27.33	A
	MOTA	1687	N	SER	319	32.618	91.790	13.406	1.00 23.18	A

	ATOM	1688	H SER	319	33.278	92.338	12.932	1.00 0.00	A
	ATOM	1689	CA SER	319	32.261	92.198	14.757	1.00 22.35	A
	ATOM	1690	CB SER	319	32.972	93.523	15.071	1.00 21.96	A
_	ATOM	1691	OG SER	319	33.554	93.517	16.360	1.00 35.71	A
5	ATOM	1692	HG SER	319	34.201	92.809	16.416	1.00 0.00	A
	ATOM	1693	C SER	319	30.765	92.371	14.988	1.00 22.88	A
	ATOM ATOM	1694 1695	O SER N ASP	319 320	30.212 30.128	91.854 93.157	15.959 14.125	1.00 20.95 1.00 25.15	A A
	ATOM	1696	H ASP	320	30.632	93.579	13.399	1.00 0.00	A
10	ATOM	1697	CA ASP	320	28.698	93.400	14.232	1.00 23.64	A
	ATOM	1698	CB ASP	320	28.383	94.447	15.334	1.00 30.33	A
	ATOM	1699	CG ASP	320	29.128	95.762	15.156	1.00 27.91	A
	ATOM	1700	OD1 ASP	320	30.369	95.774	15.088	1.00 27.84	A
. ~	MOTA	1701	OD2 ASP	320	28.456	96.799	15.098	1.00 30.37	A
15	ATOM	1702	C ASP	320	28.093	93.791	12.896	1.00 21.79	A
	ATOM ATOM	1703 1704	O ASP N GLU	320 321	28.796 26.781	93.896 93.982	11.893 12.878	1.00 21.85 1.00 23.98	A A
	ATOM	1704	H GLU	321	26.274	93.890	13.711	1.00 23.98	A
	ATOM	1706	CA GLU	321	26.077	94.326	11.652	1.00 25.27	A
20	ATOM	1707	CB GLU	321	24.565	94.361	11.920	1.00 24.89	A
	ATOM	1708	CG GLU	321	23.954	92.980	12.285	1.00 16.77	A
	MOTA	1709	CD GLU	321	23.945	92.711	13.793	1.00 16.37	A
	ATOM	1710	OE1 GLU	321	24.672	93.402	14.533	1.00 17.10	A
25	MOTA	1711 1712	OE2 GLU	321 321	23.203 26.547	91.815 95.638	14.244 $11.019$	1.00 21.60 1.00 30.46	A A
23	ATOM ATOM	1713	C GLU O GLU	321	26.547	95.733	9.795	1.00 30.46	A
	MOTA	1714	N LEU	322	26.804	96.649	11.847	1.00 20.02	A
	ATOM	1715	H LEU	322	26.680	96.524	12.809	1.00 0.00	A
	MOTA	1716	CA LEU	322	27.266	97.937	11.338	1.00 33.52	A
30	ATOM	1717	CB LEU	322	27.371	98.959	12.480	1.00 24.65	A
	ATOM	1718	CG LEU	322	26.103	99.774	12.671	1.00 21.95	A
	ATOM ATOM	1719 1720	CD1 LEU CD2 LEU	322 322	26.344 25.653	100.939 100.267	13.616 11.323	1.00 25.01 1.00 29.24	A A
	ATOM	1721	C LEU	322	28.620	97.824	10.632	1.00 25.24	A
35	ATOM	1722	O LEU	322	28.860	98.497	9.630	1.00 38.95	A
	ATOM	1723	N ALA	323	29.492	96.962	11.142	1.00 35.14	A
	MOTA	1724	H ALA	323	29.236	96.426	11.923	1.00 0.00	A
	ATOM	1725	CA ALA	323	30.826	96.790	10.569	1.00 35.03	A
40	MOTA	1726 1727	CB ALA C ALA	323 323	31.768 30.880	96.217 95.925	11.625 9.311	1.00 35.40 1.00 35.38	A A
40	ATOM ATOM	1728	C ALA O ALA	323	31.967	95.531	8.878	1.00 33.38	A
	ATOM	1729	N LEU	324	29.718	95.632	8.730	1.00 33.27	A
	ATOM	1730	H LEU	324	28.891	95.981	9.121	1.00 0.00	A
	ATOM	1731	CA LEU	324	29.638	94.805	7.525	1.00 30.65	A
45	ATOM	1732	CB LEU	324	28.199	94.313	7.308	1.00 28.08	A
	MOTA	1733 1734	CG LEU CD1 LEU	324 324	27.672 26.168	92.979 92.949	7.874 7.666	1.00 27.13 1.00 24.21	A A
	MOTA MOTA	1735	CD1 LEU	324	28.304	91.773	7.178	1.00 24.21	A
	ATOM	1736	C LEU	324	30.086	95.604	6.296	1.00 37.04	A
50	ATOM	1737	O LEU	324	30.858	95.116	5.471	1.00 31.90	A
	ATOM	1738	N VAL	325	29.601	96.841	6.193	1.00 40.73	A
	ATOM	1739	H VAL	325	29.010	97.174	6.898	1.00 0.00	A
	MOTA	1740	CA VAL	325	29.923	97.711 98.996	5.069	1.00 43.41 1.00 46.34	A
55	ATOM ATOM	$1741 \\ 1742$	CB VAL CG1 VAL	325 325	29.063 27.959	98.896	5.093 4.052	1.00 46.34	A A
55	ATOM	1743	CG2 VAL	325	28.470	99.209	6.474	1.00 51.12	A
	ATOM	1744	C VAL	325	31.395	98.107	4.985	1.00 46.86	A
	ATOM	1745	O VAL	325	31.759	99.028	4.248	1.00 48.27	A
	MOTA	1746	N THR	326	32.241	97.409	5.736	1.00 45.92	A
60	ATOM	1747	H THR	326	31.892	96.697	6.310	1.00 0.00	A
	MOTA	1748	CA THR CB THR	326 326	33.672 34.180	97.677 98.101	5.729 7.125	1.00 48.06 1.00 49.74	A
	MOTA MOTA	1749 1750	CB THR OG1 THR	326	34.100	96.101	7.123	1.00 49.74	A A
	ATOM	1751	HG1 THR	326	33.943	96.315	7.928	1.00 0.00	A
65	ATOM	1752	CG2 THR	326	33.063	98.756	7.926	1.00 52.68	A
	ATOM	1753	C THR	326	34.411	96.415	5.313	1.00 47.66	A
	MOTA	1754	O THR	326	35.615	96.290	5.523	1.00 45.71	A
	ATOM	1755	N ILE	327	33.675	95.479	4.725	1.00 50.08	A
70	MOTA	1756	H ILE	327	32.720	95.648	4.586	1.00 0.00	A
70	MOTA MOTA	1757 1758	CA ILE CB ILE	327 327	34.239 33.653	94.211 93.029	4.278 5.118	1.00 49.17 1.00 46.23	A A
	ATOM	1759	CG2 ILE	327	32.917	92.026	4.237	1.00 40.23	A
	ATOM	1760	CG2 ILE	327	34.779	92.352	5.895	1.00 47.00	A
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ATOM 1771 O VAL 328 33.974 94.456 -1.252 1.00 53.08 A ATOM 1772 N LYS 329 35.114 95.745 0.190 1.00 56.00 A ATOM 1773 H LYS 329 35.130 96.192 1.061 1.00 50.00 A ATOM 1775 CB LYS 329 35.130 96.192 1.061 1.00 50.00 A ATOM 1775 CB LYS 329 37.185 96.192 1.0051 1.00 54.78 A ATOM 1776 CB LYS 329 37.185 96.192 1.00 59.48 A ATOM 1777 CD LYS 329 37.185 98.218 -1.130 1.00 62.07 A ATOM 1777 CD LYS 329 35.950 99.103 -0.777 1.00 64.89 A ATOM 1778 CB LYS 329 34.655 98.580 -1.372 1.00 68.36 A ATOM 1779 NZ LYS 329 35.400 96.815 -2.184 1.00 0.00 A ATOM 1780 HZI LYS 329 35.400 96.815 -2.184 1.00 0.00 A ATOM 1781 HZZ LYS 329 35.400 96.815 -2.184 1.00 0.00 A ATOM 1782 HZ3 LYS 329 35.935 98.117 -3.268 1.00 0.00 A ATOM 1784 O LYS 329 37.053 98.117 -3.268 1.00 0.00 A ATOM 1786 HZ LYS 329 37.053 98.117 -3.268 1.00 0.00 A ATOM 1786 HZ LYS 329 37.053 98.103 -0.781 1.00 52.46 A ATOM 1786 HZ LYS 329 37.053 98.103 -0.981 1.00 52.46 A ATOM 1786 A LA 330 36.95 94.565 -0.841 1.00 52.46 A ATOM 1786 B ALA 330 36.95 94.565 -0.841 1.00 52.46 A ATOM 1786 B ALA 330 36.95 94.257 -1.134 1.00 52.46 A ATOM 1786 B ALA 330 38.085 92.663 0.264 1.00 46.18 A ATOM 1787 CA ALA 330 38.085 92.663 0.264 1.00 46.18 A ATOM 1788 CB ALA 330 38.085 92.663 0.264 1.00 46.18 A ATOM 1790 O ALA 330 37.299 91.476 -0.287 1.00 47.64 A ATOM 1791 N LEU 331 35.984 91.484 -0.089 1.00 49.91 A ATOM 1797 CDZ LEU 331 35.984 91.844 -0.089 1.00 49.91 A ATOM 1797 CDZ LEU 331 35.984 91.845 -0.260 1.00 47.64 A ATOM 1799 C ALA 330 37.299 91.476 -0.287 1.00 47.64 A ATOM 1799 C LEU 331 35.984 91.894 -0.498 1.00 49.91 A ATOM 1799 C LEU 331 35.984 91.894 -0.498 1.00 49.91 A ATOM 1799 C DE LEU 331 35.984 91.894 -0.498 1.00 49.91 A ATOM 1799 C LEU 331 35.986 91.895 -2.817 1.00 41.67 A ATOM 1800 C GLU 333 35.985 91.896 -9.4565 1.00 44.75 A ATOM 1800 C GLU 333 35.985 91.896 -9.4565 1.00 44.75 A ATOM 1800 C GLU 333 35.985 91.896 -9.4565 1.00 44.75 A ATOM 1800 C GLU 333 35.985 91.896 -9.4565 1.00 44.75 A ATOM 1800 C GLU 333 36.985 92.506 -9.898 1.00 49.91 A ATOM 1800 C GLU 333 36.986 92.500 -9.898 1											
*** ATOM** 1764 N. VAL. 328 33.214 93.026 2.179 1.00 50.93 Å ATOM** 1765 P. VAL. 328 33.014 95.020 2.200 1.00 49.92 Å ATOM** 1766 CA VAL. 328 33.014 95.020 2.765 1.00 0.00 Å AATOM** 1766 CB VAL. 328 31.947 96.172 0.479 1.00 53.12 Å ATOM** 1766 CB VAL. 328 31.947 96.172 0.479 1.00 53.12 Å ATOM** 1766 CG VAL. 328 31.947 96.172 0.479 1.00 53.19 Å ATOM** 1769 CG2 VAL. 328 30.573 95.931 1.005 1.05 3.91 Å ATOM** 1770 C VAL. 328 31.947 95.102 1.005 1.00 53.91 Å ATOM** 1770 C VAL. 328 32.552 97.465 1.000 1.00 52.78 Å ATOM** 1771 C VAL. 328 33.914 95.043 -0.173 1.00 54.61 Å ATOM** 1772 N LYS 329 36.160 95.043 -0.173 1.00 54.61 Å ATOM** 1772 N LYS 329 36.160 95.045 1.000 1.00 52.78 Å ATOM** 1773 LYS 329 36.160 95.052 1.000 1.00 50.00 Å Å ATOM** 1775 CG LYS 329 36.160 95.052 1.000 1.00 50.00 Å Å ATOM** 1775 CG LYS 329 36.160 95.052 1.000 1.00 59.48 Å ATOM** 1777 CG LYS 329 36.160 95.052 1.000 1.00 59.48 Å ATOM** 1777 CG LYS 329 35.950 99.103 -0.777 1.00 68.36 Å ATOM** 1777 CG LYS 329 35.950 99.103 -0.777 1.00 64.89 Å ATOM** 1777 CG LYS 329 35.950 99.103 -0.777 1.00 64.89 Å ATOM** 1778 CE LYS 329 35.950 99.103 -0.777 1.00 64.89 Å ATOM** 1778 CE LYS 329 35.950 99.103 -0.777 1.00 68.36 Å ATOM** 1788 CE LYS 329 35.340 96.815 -2.194 1.00 0.00 Å ATOM** 1788 CE LYS 329 35.340 96.815 -2.194 1.00 0.00 Å ATOM** 1788 CE LYS 329 37.955 99.103 -0.377 1.00 68.36 Å ATOM** 1788 CE LYS 329 37.955 99.103 -0.377 1.00 68.36 Å ATOM** 1788 CE LYS 329 37.955 99.103 -0.377 1.00 68.36 Å ATOM** 1788 CE LYS 329 37.955 99.103 -0.377 1.00 68.36 Å ATOM** 1788 CE LYS 329 37.955 99.103 -0.277 1.00 68.36 Å ATOM** 1788 CE LYS 329 37.955 99.103 -0.277 1.00 68.36 Å ATOM** 1789 CE LYS 329 37.955 99.103 -0.277 1.00 68.36 Å ATOM** 1789 CE LYS 329 37.955 99.103 -0.277 1.00 68.36 Å ATOM** 1789 CE LYS 329 37.955 99.103 -0.277 1.00 68.36 Å ATOM** 1789 CE LYS 329 37.955 99.103 -0.270 0.00 0.00 Å ATOM** 1789 CE LYS 329 37.955 99.103 -0.270 0.00 0.00 Å ATOM** 1789 CE LYS 329 37.955 99.103 -0.270 0.00 0.00 Å ATOM** 1789 CE LYS 329 37.955 99.103 -0.270 0.00 0.00 Å ATOM		ATOM	1761	CD1	ILE	327		91.201	6.768	1.00 44.14	A
NOTION   1764   N VAL   328   33.261   95.020   2.220   1.00   49.92   A ATOM   1766   CA VAL   328   33.2878   94.998   0.812   1.00   53.12   A ATOM   1766   CA VAL   328   32.878   94.998   0.812   1.00   53.12   A ATOM   1766   CA VAL   328   31.947   96.172   0.479   1.00   51.75   A ATOM   1769   CG VAL   328   32.578   95.931   1.085   1.00   52.78   A ATOM   1770   C VAL   328   34.045   95.943   -0.173   1.005   52.78   A ATOM   1771   C VAL   328   33.974   94.456   -1.252   1.00   53.08   A ATOM   1771   C VAL   328   33.974   94.456   -1.252   1.00   53.08   A ATOM   1772   N LIVS   328   33.914   94.456   -1.252   1.00   53.08   A ATOM   1772   N LIVS   329   36.262   94.655   -1.052   -1.00   1.00   54.08   A ATOM   1774   N LIVS   329   36.262   94.655   -1.091   1.00   54.08   A ATOM   1775   CB LIVS   329   37.185   98.218   -1.130   1.00   54.08   A ATOM   1776   CB LIVS   329   37.185   98.218   -1.130   1.00   54.08   A ATOM   1777   CD LIVS   329   34.651   98.800   -1.777   1.00   62.07   A ATOM   1777   CD LIVS   329   34.651   98.800   -1.777   1.00   68.36   A ATOM   1779   NZ LIVS   329   34.651   98.800   -1.777   1.00   64.48   A ATOM   1779   NZ LIVS   329   35.410   98.805   -1.272   1.00   50.00   A ATOM   1780   HZ LIVS   329   35.410   98.805   -1.272   1.00   50.00   A ATOM   1780   HZ LIVS   329   35.410   98.805   -1.272   1.00   50.468   A ATOM   1780   HZ LIVS   329   35.410   98.805   -1.272   1.00   68.35   A ATOM   1780   HZ LIVS   329   37.053   98.515   -1.282   1.00   0.00   A ATOM   1780   HZ LIVS   329   37.053   98.516   -0.876   1.00   0.00   A ATOM   1780   HZ LIVS   329   37.053   98.505   -0.841   1.00   52.46   A ATOM   1780   HZ LIVS   329   37.053   98.505   -0.841   1.00   52.46   A ATOM   1780   HZ LIVS   329   37.053   98.505   -0.841   1.00   52.46   A ATOM   1780   HZ LIVS   329   37.053   98.505   -0.841   1.00   52.46   A ATOM   1780   HZ LIVS   329   37.053   98.505   -0.865   -0.861   -0.865   A ATOM   1780   CLUS   LIVS   330   33.935   99.117		MOTA									
Name											
ATOM	_										
ATOM   1767   CB   VAL   328   31.947   96.172   0.479   1.00   51.75   A   ATOM   1768   CG1   VAL   328   30.573   95.931   1.085   1.00   53.91   A   ATOM   1769   CG2   VAL   328   34.045   95.043   -0.173   1.00   54.61   A   ATOM   1771   O   VAL   328   34.045   95.043   -0.173   1.00   54.61   A   ATOM   1771   O   VAL   328   34.045   95.043   -0.173   1.00   54.61   A   ATOM   1771   O   VAL   328   33.974   95.745   0.190   1.00   54.08   A   ATOM   1773   H   LYS   329   35.114   95.745   0.190   1.00   54.08   A   ATOM   1774   CA   LYS   329   35.130   96.192   1.061   1.00   50.00   A   ATOM   1775   CB   LYS   329   37.185   96.987   -0.239   1.00   59.48   A   ATOM   1776   CG   LYS   329   37.185   98.218   -1.130   1.00   62.07   A   ATOM   1777   CD   LYS   329   37.185   99.218   -1.130   1.00   62.07   A   ATOM   1778   CE   LYS   329   34.655   99.103   -0.777   1.00   64.89   A   A   A   A   A   A   A   A   A	3										
ATOM   1768   CG1 VAL   328   30.573   95.931   1.085   1.00   53.91   A   A   A   A   A   A   A   A   A											
ATOM 1769 CG2 VAL 328 32.552 97.465 1.000 1.00 52.78 A ATOM 1771 C VAL 328 34.045 95.043 -0.173 1.00 54.61 A ATOM 1771 N LYS 329 35.114 95.745 0.190 1.00 56.00 A ATOM 1773 H LYS 329 35.114 95.745 0.190 1.00 56.00 A ATOM 1773 H LYS 329 35.130 96.192 1.061 1.00 0.00 A ATOM 1775 CB LYS 329 35.130 96.192 1.061 1.00 56.00 A ATOM 1776 CB LYS 329 37.185 96.192 1.0051 1.00 56.00 A ATOM 1777 CD LYS 329 37.185 96.287 -0.239 1.00 59.48 A ATOM 1777 CD LYS 329 37.185 98.218 -1.130 1.00 62.07 A ATOM 1778 CB LYS 329 37.185 98.218 -1.130 1.00 62.07 A ATOM 1778 CB LYS 329 34.651 98.580 -1.372 1.00 68.36 A ATOM 1778 NZ LYS 329 34.651 98.580 -1.372 1.00 68.36 A ATOM 1780 HZI LYS 329 35.400 96.815 -2.184 1.00 0.00 A ATOM 1780 HZI LYS 329 35.400 96.815 -2.184 1.00 0.00 A ATOM 1780 HZI LYS 329 35.385 98.117 -3.268 1.00 0.00 A ATOM 1782 HZZ LYS 329 37.053 98.117 -3.268 1.00 0.00 A ATOM 1783 C LYS 329 37.053 98.117 -3.268 1.00 0.00 A ATOM 1784 O LYS 329 37.053 98.117 -3.268 1.00 0.00 A ATOM 1784 O LYS 329 37.053 98.107 -0.194 1.00 52.66 A ATOM 1785 R ALA 330 36.995 94.257 -0.194 1.00 52.66 A ATOM 1786 HZ LYS 329 37.053 98.107 -0.195 1.00 51.87 A ATOM 1786 R ALA 330 36.995 94.257 -1.134 1.00 52.66 A ATOM 1787 CA ALA 330 36.995 94.257 -1.134 1.00 52.66 A ATOM 1786 B ALA 330 36.995 94.257 -1.134 1.00 52.66 A ATOM 1787 CA ALA 330 36.995 94.257 -1.134 1.00 52.66 A ATOM 1789 C ALA 330 37.320 93.002 0.280 1.00 47.07 A ATOM 1797 CD LEU 331 35.578 92.237 0.390 1.00 47.07 A ATOM 1797 CD LEU 331 33.355 99.248 91.60 0.266 1.00 46.08 A ATOM 1798 C LEU 331 35.578 92.237 0.390 1.00 0.70 4.00 A ATOM 1799 C LEU 331 35.578 92.237 0.390 1.00 0.70 4.00 A ATOM 1797 CD LEU 331 33.993 92.237 0.390 1.00 0.00 A ATOM 1798 C LEU 331 33.958 92.237 0.390 1.00 0.00 A ATOM 1799 C LEU 331 33.958 92.237 0.390 1.00 0.70 4.65 A ATOM 1800 C GLEU 331 33.958 92.237 0.390 1.00 0.70 4.65 A ATOM 1801 C GLEU 331 33.958 92.237 0.390 1.00 0.00 A ATOM 1803 C GLEU 333 36.995 94.257 0.390 1.00 0.00 A ATOM 1800 C GLEU 333 36.995 94.257 0.390 1.00 0.00 A ATOM 1800 C GLEU 333 36.995											
100											
APOM   1772   N   LYS   329   35.114   95.745   0.190   1.00   56.00   A   APOM   1773   H   LYS   329   35.130   96.192   1.061   1.00   0.00   A   APOM   1774   CA   LYS   329   35.185   96.987   -0.239   1.00   54.78   A   A   A   A   A   A   A   A   A	10									1.00 54.61	A
ATOM 1773 H LYS 329 35.130 96.192 1.061 1.00 0.00 0.00 A ATOM 1775 CB LYS 329 37.185 96.987 -0.239 1.00 59.48 A ATOM 1776 CG LYS 329 37.185 96.987 -0.239 1.00 59.48 A ATOM 1777 CD LYS 329 37.185 98.181 -1.130 1.00 62.07 A ATOM 1777 CD LYS 329 35.950 99.103 -0.777 1.00 64.89 A ATOM 1778 CE LYS 329 34.651 98.580 -1.372 1.00 68.36 A ATOM 1779 NZ LYS 329 34.865 97.635 -2.509 1.00 71.98 A ATOM 1780 HZZ LYS 329 34.865 97.635 -2.509 1.00 71.98 A ATOM 1781 HZZ LYS 329 35.385 98.117 -3.268 1.00 0.00 A ATOM 1782 HZZ LYS 329 35.385 98.117 -3.268 1.00 0.00 A ATOM 1782 HZZ LYS 329 37.053 94.565 -0.841 1.00 0.00 A ATOM 1784 HZZ LYS 329 37.053 94.565 -0.841 1.00 51.87 A ATOM 1785 N ALA 330 37.320 93.902 0.280 1.00 47.32 A ATOM 1786 ALA 330 36.985 92.663 0.264 1.00 47.32 A ATOM 1788 CB ALA 330 38.885 92.663 0.264 1.00 4.73 A ATOM 1788 CB ALA 330 38.885 92.663 0.264 1.00 4.73 A ATOM 1788 CB ALA 330 38.885 92.663 0.264 1.00 4.75 A ATOM 1789 C ALA 330 38.885 92.663 0.264 1.00 4.76 A ATOM 1789 C B ALA 330 38.799 91.476 -0.287 1.00 47.64 A ATOM 1799 O ALA 330 37.299 91.476 -0.287 1.00 47.64 A ATOM 1799 C B LEU 331 35.984 91.484 -0.089 1.00 42.75 A ATOM 1799 C B LEU 331 35.984 91.484 0.089 1.00 49.91 A ATOM 1799 C B LEU 331 35.984 91.484 0.089 1.00 49.91 A ATOM 1799 C B LEU 331 35.984 91.484 0.089 1.00 49.91 A ATOM 1799 C B LEU 331 35.125 90.398 -0.568 1.00 47.07 A ATOM 1799 C B LEU 331 33.395 88.085 92.877 0.138 1.00 48.89 A ATOM 1799 C B LEU 331 33.395 88.085 92.477 0.390 1.00 0.00 A ATOM 1799 C B LEU 331 33.395 88.085 92.877 0.398 1.00 40.91 A ATOM 1799 C B LEU 331 33.395 88.085 92.877 0.398 1.00 40.91 A ATOM 1799 C B LEU 331 33.395 88.085 92.877 0.398 1.00 40.91 A ATOM 1799 C B LEU 331 33.395 88.085 92.877 0.398 1.00 44.64 A ATOM 1800 R GLY 332 34.682 92.530 -1.800 1.00 47.55 A ATOM 1807 C A G G LEU 331 33.395 88.028 9.495 1.00 42.75 A ATOM 1807 C A G G LEU 331 33.395 88.028 9.495 1.00 42.75 A ATOM 1807 C A G G LEU 331 33.395 88.028 9.495 1.00 42.75 A ATOM 1807 C A G G LEU 331 33.395 88.028 9.495 1.00 37.35 A ATOM 1807 C A G G G		MOTA	1771	0 '	VAL	328	33.974		-1.252	1.00 53.08	A
ATOM 1774 CA LYS 329 36.262 95.855 -0.699 1.00 54.78 A ATOM 1775 CG LYS 329 37.135 98.218 -1.130 1.00 62.07 A ATOM 1776 CG LYS 329 37.135 98.218 -1.130 1.00 62.07 A ATOM 1777 CD LYS 329 35.950 99.103 -0.777 1.00 64.89 A ATOM 1778 CE LYS 329 34.651 98.586 -1.372 1.00 68.36 A ATOM 1779 DZ LYS 329 34.651 98.586 -1.372 1.00 68.36 A ATOM 1780 HZL LYS 329 35.410 96.815 -2.184 1.00 0.00 A ATOM 1781 HZZ LYS 329 35.410 96.815 -2.184 1.00 0.00 A ATOM 1781 HZZ LYS 329 35.410 96.815 -2.184 1.00 0.00 A ATOM 1781 HZZ LYS 329 35.410 96.815 -2.184 1.00 0.00 A ATOM 1782 HZ3 LYS 329 35.420 96.815 -2.184 1.00 0.00 A ATOM 1783 CLYS 329 37.406 94.173 -1.954 1.00 52.46 A ATOM 1784 O LYS 329 37.406 94.173 -1.954 1.00 52.46 A ATOM 1785 A ATOM 1786 H ALA 330 36.995 94.257 1.134 1.00 52.46 A ATOM 1787 CA ALA 330 36.995 94.257 1.134 1.00 52.46 A ATOM 1788 CB ALA 330 37.20 93.902 0.280 1.00 47.32 A ATOM 1789 CB ALA 330 38.581 92.348 1.659 1.00 42.75 A ATOM 1790 O ALA 330 37.877 90.567 -0.876 1.00 42.75 A ATOM 1790 C ALA 330 37.877 90.567 -0.876 1.00 42.76 A ATOM 1790 C ALA 330 37.877 90.567 -0.876 1.00 42.76 A ATOM 1790 C ALA 330 37.877 90.567 -0.876 1.00 47.07 A ATOM 1790 C ALA 331 35.578 92.237 0.390 1.00 47.07 A ATOM 1790 C ALE 331 35.578 92.237 0.390 1.00 47.07 A ATOM 1790 C ALE 331 35.578 92.237 0.390 1.00 40.90 A ATOM 1790 C ALE 331 35.578 92.237 0.390 1.00 40.707 A ATOM 1790 C ALE 331 35.578 92.237 0.390 1.00 40.707 A ATOM 1790 C ALE 331 35.578 92.237 0.390 1.00 40.707 A ATOM 1790 C ALE 331 35.578 92.237 0.390 1.00 40.707 A ATOM 1800 C GLU 331 35.578 92.237 0.390 1.00 40.707 A ATOM 1790 C ALE 331 35.578 92.237 0.390 1.00 40.707 A ATOM 1790 C ALE 331 35.578 92.237 0.390 1.00 40.707 A ATOM 1800 C GLU 331 33.368 98.91 89.568 1.00 46.71 A ATOM 1800 C GLU 333 36.898 91		MOTA									
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ATOM 1831 O ARG 334 38 181 86.231 -4 788 1 00 40 32 A	70	ATOM	1830	C	ARG						
		MOTA	1831		ARG	334	38.181	86.231	-4.788	1.00 40.32	A
ATOM 1832 N ILE 335 36.662 87.903 -4.748 1.00 44.23 A											
ATOM 1833 H ILE 335 36.458 88.813 -4.452 1.00 0.00 A		ATOM	1833	н	TTT	333	J0.458	00.813	-4.402	1.00 0.00	A

	ATOM	1834	CA	ILE	335	35.663	87.164	-5.504	1.00 45.07	A
	ATOM	1835	CB I	ILE	335	34.260	87.798	-5.329	1.00 46.64	A
	MOTA	1836	CG2	ILE	335	34.330	89.285	-5.585	1.00 50.46	A
	ATOM	1837	CG1	ILE	335	33.254	87.149	-6.283	1.00 50.93	A
5	MOTA	1838	CD1		335	33.110	85.645	-6.114	1.00 53.73	A
	ATOM	1839		ILE	335	36.045	87.134	-6.977	1.00 41.85	A
	ATOM	1840		ILE	335	36.246	86.070	-7.547	1.00 44.44	A
	ATOM	1841		PHE	336	36.159	88.304	-7.591	1.00 38.93	A
10	ATOM	1842		PHE	336 336	35.995 36.526	89.130 88.371	-7.093 -8.994	1.00 0.00 1.00 40.81	A A
10	ATOM ATOM	1843 1844		PHE PHE	336	36.041	89.684	-9.590	1.00 40.81	A
	ATOM	1845		PHE	336	34.548	89.816	-9.618	1.00 30.97	A
	MOTA	1846	CD1		336	33.895	90.694	-8.753	1.00 30.10	A
	ATOM	1847	CD2		336	33.792		-10.513	1.00 29.08	A
15	MOTA	1848	CE1		336	32.513	90.821	-8.783	1.00 15.73	A
	MOTA	1849		PHE	336	32.409	89.197		1.00 19.75	A
	MOTA	1850		PHE	336	31.772	90.078	-9.677	1.00 20.19	A
	MOTA	1851		PHE	336	38.035	88.240	-9.188	1.00 41.18	A
20	MOTA	1852		PHE	336	38.463		-10.356	1.00 41.37	A
20	ATOM	1853 1854		PHE ALA	336 145	38.771 27.124	88.233 80.130	-8.178 34.005	1.00 40.25 1.00 39.54	A B
	ATOM ATOM	1855		ALA	145	25.323	81.127	32.585	1.00 33.34	В
	ATOM	1856		ALA	145	24.364	80.726	33.254	1.00 37.41	B
	ATOM	1857	HT1		145	26.147	82.508	34.837	1.00 0.00	В
25	ATOM	1858	HT2 2		145	26.612	83.408	33.474	1.00 0.00	В
	MOTA	1859		ALA	145	26.822	82.567	34.050	1.00 42.77	В
	MOTA	1860	HT3 2		145	27.790	82.642	34.428	1.00 0.00	В
	ATOM	1861		ALA	145	26.715	81.343	33.203	1.00 39.62	В
30	MOTA	1862		GLN	146	25.236 26.034	81.388 81.700	31.288 30.819	1.00 33.32 1.00 0.00	B B
30	ATOM ATOM	1863 1864		GLN GLN	146 146	24.004	81.230	30.537	1.00 31.87	В
	ATOM	1865		GLN	146	24.024	82.162	29.354	1.00 29.22	В
	ATOM	1866		GLN	146	23.274	83.421	29.543	1.00 34.86	В
	ATOM	1867		GLN	146	23.349	84.236	28.288	1.00 39.34	В
35	ATOM	1868	OE1 (	GLN	146	24.442	84.554	27.821	1.00 41.32	В
	ATOM	1869	NE2		146	22.200	84.559	27.720	1.00 38.82	В
	ATOM		HE21 (		146	21.354	84.268	28.120	1.00 0.00	В
	ATOM		HE22		146 146	22.239 23.862	85.092 79.804	26.900 30.023	1.00 0.00 1.00 27.45	B B
40	MOTA MOTA	1872 1873		GLN GLN	146	24.525	79.400	29.079	1.00 27.43	В
10	MOTA	1874		LEU	147	22.965	79.050	30.622	1.00 27.23	В
	ATOM	1875		LEU	147	22.423	79.419	31.350	1.00 0.00	В
	ATOM	1876	CA I	LEU	147	22.776	77.675	30.211	1.00 28.64	В
	MOTA	1877		LEU	147	23.538	76.760	31.165	1.00 27.79	В
45	ATOM	1878		LEU	147	24.667	75.818	30.759	1.00 27.05	В
	MOTA	1879	CD1		147	25.208 25.742	76.106 75.956	29.374 31.812	1.00 24.90 1.00 24.14	B B
	MOTA MOTA	1880 1881	CD2 :	LEU	147 147	21.302	77.303	30.261	1.00 24.14	В
	MOTA	1882		LEU	147	20.576	77.731	31.150	1.00 25.85	В
50	ATOM	1883		ASP	148	20.872	76.502	29.297	1.00 27.82	В
	MOTA	1884		ASP	148	21.489	76.235	28.585	1.00 0.00	В
	MOTA	1885	CA	ASP	148	19.506	76.019	29.279	1.00 22.46	В
	MOTA	1886		ASP	148	18.920	76.112	27.881	1.00 20.10	В
55	MOTA	1887		ASP	148	18.424	77.504	27.561 26.375	1.00 12.21 1.00 14.78	В
55	MOTA	1888	OD1 A		148 148	18.422	77.881 78.216	28.494	1.00 14.78	B B
	ATOM ATOM	1889 1890		ASP ASP	148	18.040 19.703	74.568	29.680	1.00 13.38	В
	ATOM	1891		ASP	148	20.389	73.822	28.986	1.00 23.66	В
	ATOM	1892		ILE	149	19.138	74.190	30.822	1.00 17.82	В
60	MOTA	1893		ILE	149	18.603	74.833	31.327	1.00 0.00	В
	MOTA	1894		ILE	149	19.296	72.838	31.332	1.00 14.75	В
	MOTA	1895		ILE	149	19.901	72.847	32.752	1.00 15.94	В
	MOTA	1896		ILE	149	20.143	71.431	33.218	1.00 8.68	В
65	ATOM	1897	CG1		149	21.192 21.672	73.685 73.954	32.788 34.217	1.00 13.92 1.00 7.01	B B
03	ATOM	1898 1899	CD1 C	ILE	149 149	17.977	72.076	31.427	1.00 19.66	В
	ATOM ATOM	1900		ILE	149	16.969	72.581	31.935	1.00 17.11	В
	ATOM	1901		VAL	150	18.008	70.843	30.959	1.00 15.39	В
	ATOM	1902		VAL	150	18.833	70.497	30.565	1.00 0.00	В
70	MOTA	1903	CA .	VAL	150	16.847	69.992	31.017	1.00 14.24	В
	MOTA	1904		VAL	150	16.399	69.565	29.612	1.00 18.62	В
	ATOM	1905	CG1		150	15.323	68.478	29.707	1.00 11.48 1.00 14.10	B B
	ATOM	1906	CG2	٧AL	150	15.861	70.773	28.869	1.00 14.10	а

	ATOM	1907	С	VAL	150	17.193	68.760	31.837	1.00 13.47	В
	ATOM	1908	Ō	VAL	150	18.166	68.050	31.558	1.00 16.28	В
	ATOM	1909	N	ILE	151	16.390	68.534	32.864	1.00 13.89	В
	MOTA	1910	H	ILE	151	15.666	69.164	33.048	1.00 0.00	В
5	MOTA	1911	CA	ILE	151	16.554	67.384	33.725	1.00 12.32	В
0	ATOM	1912	CB	ILE	151	16.146	67.712	35.160	1.00 12.32	В
	ATOM	1913	CG2	ILE	151	16.359	66.524	36.033	1.00 4.81	В
		1914		ILE						
	MOTA		CG1		151	16.907	68.934	35.668	1.00 15.50	В
10	ATOM	1915	CD1	ILE	151	16.390	69.451	37.017	1.00 16.51	В
10	MOTA	1916	C	ILE	151	15.625	66.309	33.174	1.00 12.57	В
	ATOM	1917	0	ILE	151	14.448	66.548	32.988	1.00 15.95	В
	MOTA	1918	N	VAL	152	16.184	65.141	32.869	1.00 16.00	В
	ATOM	1919	H	VAL	152	17.150	65.032	32.993	1.00 0.00	В
	ATOM	1920	CA	VAL	152	15.410	64.009	32.354	1.00 14.98	В
15	ATOM	1921	CB	VAL	152	16.082	63.397	31.106	1.00 15.24	В
	ATOM	1922	CG1	VAL	152	15.209	62.279	30.531	1.00 10.15	В
	ATOM	1923	CG2	VAL	152	16.313	64.500	30.056	1.00 7.29	В
	ATOM	1924	С	VAL	152	15.438	63.052	33.532	1.00 19.19	В
	ATOM	1925	0	VAL	152	16.459	62.414	33.835	1.00 16.07	В
20	ATOM	1926	N	LEU	153	14.297	62.976	34.200	1.00 15.97	В
	ATOM	1927	Н	LEU	153	13.519	63.456	33.851	1.00 0.00	В
	ATOM	1928	CA	LEU	153	14.150	62.211	35.414	1.00 13.99	В
	ATOM	1929	CB	LEU	153	13.530	63.131	36.474	1.00 15.97	В
	ATOM	1930	CG	LEU	153	12.764	62.553	37.658	1.00 13.37	В
25	ATOM	1931		LEU	153	13.616	61.536	38.376		
23		1931							1.00 23.41	В
	ATOM		CD2	LEU	153	12.367	63.672	38.599	1.00 15.08	В
	ATOM	1933	C	LEU	153	13.362	60.924	35.309	1.00 17.91	В
	MOTA	1934	0	LEU	153	12.214	60.923	34.870	1.00 23.80	В
20	MOTA	1935	N	ASP	154	14.002	59.832	35.723	1.00 19.62	В
30	MOTA	1936	H	ASP	154	14.918	59.927	36.051	1.00 0.00	В
	ATOM	1937	CA	ASP	154	13.397	58.504	35.709	1.00 19.43	В
	ATOM	1938	CB	ASP	154	14.461	57.432	35.966	1.00 17.84	В
	ATOM	1939	CG	ASP	154	13.912	56.021	35.831	1.00 27.80	В
	ATOM	1940	OD1	ASP	154	12.725	55.871	35.461	1.00 28.40	В
35	ATOM	1941	OD2	ASP	154	14.667	55.059	36.094	1.00 28.69	В
	ATOM	1942	С	ASP	154	12.351	58.419	36.804	1.00 18.93	В
	ATOM	1943	0	ASP	154	12.698	58.429	37.993	1.00 15.86	В
	ATOM	1944	N	GLY	155	11.080	58.328	36.407	1.00 18.75	В
	ATOM	1945	H	GLY	155	10.873	58.317	35.453	1.00 0.00	В
40	ATOM	1946	CA	GLY	155	10.012	58.247	37.382	1.00 15.14	В
	MOTA	1947	C	GLY	155	9.479	56.842	37.537	1.00 19.82	В
	ATOM	1948	Ö	GLY	155	8.308	56.668	37.882	1.00 13.02	В
	ATOM	1949	N	SER	156	10.342	55.854	37.280	1.00 14.30	В
	ATOM	1950	H	SER	156	11.250	56.096	37.200	1.00 0.00	В
45	ATOM	1951			156					
43			CA	SER		10.008	54.434	37.396	1.00 17.78	В
	MOTA	1952	CB	SER	156	11.217	53.559	36.993	1.00 23.82	В
	ATOM	1953	OG	SER	156	12.195	53.479	38.040	1.00 34.45	В
	MOTA	1954	HG	SER	156	12.517	54.359	38.245	1.00 0.00	В
50	ATOM	1955	C	SER	156	9.581		38.826	1.00 14.28	В
50	MOTA	1956	0	SER	156	9.531	55.014	39.675	1.00 16.84	В
	MOTA	1957	N	ASN	157	9.298	52.866	39.113	1.00 15.15	В
	MOTA	1958	H	ASN	157	9.411	52.173	38.428	1.00 0.00	В
	MOTA	1959	CA	ASN	157	8.820	52.507	40.443	1.00 13.34	В
	MOTA	1960	CB	ASN	157	7.869	51.305	40.353	1.00 16.24	В
55	MOTA	1961	CG	ASN	157	6.634	51.580	39.529	1.00 20.72	В
	ATOM	1962	OD1	ASN	157	5.997	50.643	39.036	1.00 27.20	В
	ATOM	1963	ND2		157	6.273	52.859	39.374	1.00 18.41	В
	ATOM		HD21		157	6.805	53.570	39.787	1.00 0.00	В
	ATOM		HD22		157	5.473	53.041	38.841	1.00 0.00	В
60	ATOM	1966	C	ASN	157	9.865	52.190	41.511	1.00 16.46	В
00	ATOM	1967	0		157	9.517	52.117			D D
				ASN				42.693	1.00 20.71	В
	ATOM	1968	N	SER	158	11.127	52.030	41.132	1.00 15.18	В
	ATOM	1969	H	SER	158	11.384	52.156	40.196	1.00 0.00	В
65	ATOM	1970	CA	SER	158	12.151	51.654	42.127	1.00 16.23	В
65	ATOM	1971	CB	SER	158	13.161	50.690	41.487	1.00 13.88	В
	MOTA	1972	OG	SER	158	13.678	51.221	40.296	1.00 15.34	В
	ATOM	1973	$^{\mathrm{HG}}$	SER	158	14.121	52.052	40.478	1.00 0.00	В
	MOTA	1974	C	SER	158	12.911	52.713	42.948	1.00 17.21	В
	ATOM	1975	0	SER	158	13.395	52.397	44.046	1.00 16.37	В
70	MOTA	1976	N	ILE	159	13.061	53.938	42.446	1.00 22.58	В
	ATOM	1977	Н	ILE	159	12.726	54.145	41.550	1.00 0.00	В
	ATOM	1978	CA	ILE	159	13.733	54.975	43.241	1.00 22.49	В
	ATOM	1979	CB	ILE	159	13.674	56.360	42.566	1.00 24.48	В
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	MOTA	1980	CG2 ILE	159	14.718	57.288	43.176	1.00 24.15	В
	MOTA	1981	CG1 ILE	159	13.812	56.209	41.057	1.00 32.59	В
	ATOM	1982	CD1 ILE	159	12.470	56.393	40.303	1.00 20.06	В
_	ATOM	1983	C ILE	159	12.778	55.028	44.407	1.00 24.33	В
5	MOTA	1984	O ILE	159	11.724	55.618	44.285	1.00 17.55	В
	ATOM	1985	N TYR	160	13.099	54.420	45.541	1.00 32.15	В
	ATOM	1986	H TYR	160	13.965	53.980	45.664	1.00 0.00	В
	ATOM	1987 1988	CA TYR CB TYR	160 160	12.097 12.267	54.447 53.324	46.585 47.597	1.00 31.82 1.00 26.96	B B
10	ATOM ATOM	1989	CG TYR	160	11.253	53.490	48.725	1.00 25.65	В
10	ATOM	1990	CD1 TYR	160	9.926	53.897	48.457	1.00 24.26	В
	ATOM	1991	CE1 TYR	160	9.022	54.114	49.484	1.00 18.27	В
	ATOM	1992	CD2 TYR	160	11.623	53.306	50.041	1.00 20.35	В
	ATOM	1993	CE2 TYR	160	10.729	53.519	51.072	1.00 22.84	B
15	ATOM	1994	CZ TYR	160	9.441	53.917	50.791	1.00 14.51	В
	ATOM	1995	OH TYR	160	8.598	54.099	51.840	1.00 23.91	В
	ATOM	1996	HH TYR	160	9.063	53.916	52.661	1.00 0.00	В
	MOTA	1997	C TYR	160	11.880	55.733	47.356	1.00 37.48	В
••	MOTA	1998	O TYR	160	10.799	56.335	47.262	1.00 44.11	В
20	ATOM	1999	N PRO	161	12.855	56.167	48.158	1.00 31.96	В
	ATOM	2000	CD PRO	161	14.215	55.743	48.529	1.00 22.44	В
	MOTA	2001	CA PRO	161	12.466	57.408	48.822	1.00 28.82 1.00 31.11	B B
	ATOM ATOM	2002 2003	CB PRO	161 161	13.575 14.337	57.639 56.332	49.856 49.902	1.00 31.11	В
25	ATOM	2003	C PRO	161	12.414	58.464	47.729	1.00 23.46	В
23	ATOM	2005	O PRO	161	13.452	58.977	47.298	1.00 18.53	В
	ATOM	2006	N TRP	162	11.204	58.741	47.246	1.00 23.04	В
	ATOM	2007	H TRP	162	10.424	58.275	47.612	1.00 0.00	В
	MOTA	2008	CA TRP	162	11.019	59.719	46.184	1.00 20.85	В
30	MOTA	2009	CB TRP	162	9.565	59.743	45.720	1.00 24.84	В
	ATOM	2010	CG TRP	162	9.344	60.700	44.583	1.00 15.34	В
	MOTA	2011	CD2 TRP	162	9.779	60.531	43.229	1.00 17.68	В
	ATOM	2012	CE2 TRP	162	9.364	61.679	42.516	1.00 13.50	В
35	MOTA	2013	CE3 TRP	162	10.474	59.531	42.545	1.00 12.30	В
33	ATOM ATOM	2014 2015	CD1 TRP NE1 TRP	162 162	8.704 8.712	61.897 62.491	44.640 43.399	1.00 12.84 1.00 14.37	B B
	ATOM	2016	HE1 TRP	162	8.323	63.357	43.175	1.00 14.37	В
	ATOM	2017	CZ2 TRP	162	9.625	61.847	41.158	1.00 14.57	В
	ATOM	2018	CZ3 TRP	162	10.732	59.699	41.198	1.00 13.59	В
40	ATOM	2019	CH2 TRP	162	10.307	60.853	40.517	1.00 10.94	В
	ATOM	2020	C TRP	162	11.431	61.091	46.692	1.00 21.81	В
	ATOM	2021	O TRP	162	12.010	61.884	45.969	1.00 16.84	В
	MOTA	2022	N GLU	163	11.135	61.363	47.952	1.00 25.91	В
4	ATOM	2023	H GLU	163	10.665	60.699	48.497	1.00 0.00	В
45	MOTA	2024	CA GLU	163	11.506	62.644	48.524	1.00 33.12	В
	MOTA	2025 2026	CB GLU	163 163	11.066 11.646	62.721 61.637	49.993 50.888	1.00 36.71 1.00 47.66	B B
	ATOM ATOM	2027	CG GLU CD GLU	163	10.848	61.447	52.173	1.00 47.00	В
	ATOM	2028	OE1 GLU	163	11.446	61.522	53.270	1.00 57.76	В
50	ATOM	2029	OE2 GLU	163	9.620	61.221	52.088	1.00 59.92	В
	ATOM	2030	C GLU	163	13.013	62.848	48.418	1.00 31.56	В
	ATOM	2031	O GLU	163	13.496	63.980	48.447	1.00 28.76	В
	MOTA	2032	N SER	164	13.748	61.747	48.270	1.00 31.75	В
	ATOM	2033	H SER	164	13.295	60.879	48.215	1.00 0.00	В
55	ATOM	2034	CA SER	164	15.213	61.788	48.181	1.00 31.88	В
	ATOM	2035	CB SER	164	15.795	60.399	48.470	1.00 31.21	В
	MOTA	2036	OG SER	164 164	15.996 16.606	60.221	49.864	1.00 32.68	B B
	ATOM ATOM	2037 2038	HG SER C SER	164	15.751	60.887 62.289	50.185 46.845	1.00 0.00 1.00 29.05	В
60	ATOM	2039	O SER	164	16.820	62.890	46.782	1.00 29.91	В
00	ATOM	2040	N VAL	165	15.030	61.998	45.772	1.00 22.58	В
	ATOM	2041	H VAL	165	14.209	61.472	45.867	1.00 0.00	В
	ATOM	2042	CA VAL	165	15.443	62.454	44.462	1.00 26.86	В
	MOTA	2043	CB VAL	165	14.761	61.610	43.333	1.00 30.69	В
65	MOTA	2044	CG1 VAL	165	13.791	62.460	42.533	1.00 27.74	В
	MOTA	2045	CG2 VAL	165	15.825	61.022	42.411	1.00 33.05	В
	ATOM	2046	C VAL	165	15.029	63.926	44.386	1.00 27.11	В
	MOTA	2047	O VAL	165	15.746	64.762	43.843	1.00 23.73	В
70	ATOM	2048	N ILE	166	13.860	64.238	44.936	1.00 26.45	В
70	ATOM	2049	H ILE	166 166	13.308	63.536 65.618	45.338 44.943	1.00 0.00 1.00 21.89	B B
	ATOM ATOM	2050 2051	CA ILE CB ILE	166 166	13.388 11.931	65.706	44.943	1.00 21.89	В
	ATOM	2052	CG2 ILE	166	11.469	67.157	45.379	1.00 24.33	В
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	ATOM	2053	CG1	ILE	166	11.047	64.822	44.505	1.00 28.66	В
	MOTA	2054	CD1	ILE	166	11.350	64.929	42.999	1.00 20.77	В
	ATOM	2055	C	ILE	166	14.283	66.471	45.842	1.00 18.82	В
_	ATOM	2056	0	ILE	166	14.476	67.651	45.577	1.00 18.46 1.00 12.61	В
5	ATOM ATOM	2057 2058	N H	ALA ALA	167 167	14.828 14.615	65.882 64.949	46.904 47.105	1.00 12.61 1.00 0.00	B B
	ATOM	2059	CA	ALA	167	15.750	66.625	47.768	1.00 14.63	В
	ATOM	2060	CB	ALA	167	16.054	65.836	49.048	1.00 15.91	В
	ATOM	2061	C	ALA	167	17.045	66.847	46.961	1.00 15.69	В
10	ATOM	2062	0	ALA	167	17.647	67.906	47.036	1.00 17.79	В
	MOTA	2063	N	PHE	168	17.450	65.842	46.181	1.00 14.44	В
	ATOM	2064	H	PHE	168	16.926	65.014	46.166	1.00 0.00	В
	ATOM	2065	CA	PHE	168	18.656	65.936	45.346	1.00 14.68	В
15	ATOM	2066	CB CG	PHE PHE	168 168	18.878 19.832	64.608 64.680	44.615 $43.444$	1.00 12.59 1.00 20.18	B B
13	ATOM ATOM	2067 2068	CD1		168	19.355	64.609	42.134	1.00 20.18	В
	MOTA	2069	CD2		168	21.211	64.759	43.645	1.00 16.50	В
	ATOM	2070	CE1		168	20.226	64.606	41.047	1.00 18.84	В
	ATOM	2071	CE2	PHE	168	22.092	64.760	42.564	1.00 14.29	В
20	MOTA	2072	CZ	PHE	168	21.599	64.680	41.263	1.00 15.75	В
	MOTA	2073	C	PHE	168	18.501	67.066	44.336	1.00 17.90	В
	ATOM	2074	0	PHE	168	19.420	67.847	44.114	1.00 19.14	В
	ATOM	2075 2076	N H	LEU LEU	169 169	17.328 16.627	67.148 66.494	43.719 43.929	1.00 18.88 1.00 0.00	B B
25	ATOM ATOM	2077	СA	LEU	169	17.068	68.187	42.745	1.00 16.96	В
20	ATOM	2078	CB	LEU	169	15.779	67.885	41.984	1.00 19.20	В
	ATOM	2079	CG	LEU	169	15.843	66.692	41.022	1.00 14.34	В
	ATOM	2080	CD1	LEU	169	14.476	66.482	40.428	1.00 16.09	В
	ATOM	2081	CD2		169	16.864	66.920	39.926	1.00 14.01	В
30	ATOM	2082	C	LEU	169	16.977	69.558	43.407	1.00 19.79	В
	ATOM	2083	0	LEU	169	17.443	70.547	42.844	1.00 26.07	B B
	ATOM ATOM	2084 2085	N H	ASN ASN	170 170	16.377 16.011	69.617 68.795	44.593 44.984	1.00 21.05 1.00 0.00	В
	ATOM	2086	CA	ASN	170	16.249	70.875	45.332	1.00 22.16	В
35	ATOM	2087	CB	ASN	170	15.473	70.655	46.630	1.00 27.93	В
	ATOM	2088	CG	ASN	170	15.617	71.834	47.611	1.00 32.39	В
	MOTA	2089		ASN	170	16.661	72.003	48.257	1.00 29.22	В
	ATOM	2090		ASN	170	14.572	72.643	47.718	1.00 25.77	В
40	ATOM		HD21		170	13.765	72.473	47.191	1.00 0.00	B B
40	ATOM ATOM	2092	HD22 C	ASN	170 170	14.648 17.609	73.396 71.498	48.340 45.668	1.00 0.00	В
	ATOM	2094	0	ASN	170	17.832	72.689	45.426	1.00 24.64	В
	ATOM	2095	N	ASP	171	18.509	70.684	46.223	1.00 22.99	В
	MOTA	2096	H	ASP	171	18.262	69.748	46.378	1.00 0.00	В
45	MOTA	2097	CA	ASP	171	19.855	71.128	46.610	1.00 20.63	В
	MOTA	2098	CB	ASP	171	20.593	70.014	47.360	1.00 20.85	В
	MOTA	2099	CG	ASP	171	19.869 19.031	69.585	48.619 49.124	1.00 29.81 1.00 25.40	B B
	ATOM ATOM	2100 2101	OD1	ASP	171 171	20.131	70.371 68.465		1.00 29.96	В
50	ATOM	2102	Ç	ASP	171	20.685	71.544	45.416	1.00 22.06	В
	ATOM	2103	Õ	ASP	171	21.537	72.431	45.519	1.00 26.11	В
	MOTA	2104	N	LEU	172	20.447	70.876	44.292	1.00 19.55	В
	MOTA	2105	H	LEU	172	19.776	70.165	44.301	1.00 0.00	В
~ ~	MOTA	2106	CA	LEU	172	21.146	71.162	43.050	1.00 20.55	В
55	MOTA	2107	CB	LEU	172	20.866	70.044	42.056	1.00 25.39	В
	ATOM ATOM	2108 2109	CG CD1	LEU LEU	172 172	21.889 $21.174$	69.703 68.935	40.978 39.874	1.00 23.87 1.00 26.42	B B
	ATOM	2110		LEU	172	22.543	70.947	40.435	1.00 20.42	В
	ATOM	2111	C	LEU	172	20.697	72.484	42.428	1.00 20.44	В
60	ATOM	2112	Ō	LEU	172	21.518	73.313	42.014	1.00 21.12	В
	ATOM	2113	N	LEU	173	19.383	72.646	42.343	1.00 18.93	В
	ATOM	2114	H	LEU	173	18.803	71.938	42.694	1.00 0.00	В
	ATOM	2115	CA	LEU	173	18.761	73.826	41.755	1.00 21.30	В
65	ATOM	2116	CB	LEU	173	17.248	73.588	41.573	1.00 20.45	В
65	ATOM	2117	CG CD1	LEU	173	16.850	72.431	40.649 40.926	1.00 20.49 1.00 22.02	B B
	ATOM ATOM	2118 2119		LEU LEU	173 173	15.418 16.999	72.019 72.855	39.197	1.00 22.02	B
	ATOM	2120	CDZ	LEU	173	18.966	75.081	42.583	1.00 18.86	В
	ATOM	2121	0	LEU	173	19.266	76.146	42.046	1.00 16.41	В
70	MOTA	2122	N	LYS	174	18.799	74.953	43.894	1.00 21.55	В
	ATOM	2123	H	LYS	174	18.581	74.076	44.275	1.00 0.00	В
	MOTA	2124	CA	LYS	174	18.943	76.107	44.765	1.00 23.18	В
	ATOM	2125	CB	LYS	174	18.648	75.717	46.216	1.00 26.28	В

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	MOTA	2126	CG	LYS	174	19.830	75.202	47.026	1.00 29.25	В
	ATOM	2127	CD	LYS	174	19.306	74.550	48.304	1.00 28.29	В
	MOTA	2128	CE	LYS	174	20.399	73.886	49.111	1.00 19.54	В
_	ATOM	2129	NZ	LYS	174	19.815	73.374	50.359	1.00 21.14	В
5	ATOM	2130	HZ1		174	19.069	72.682 74.161	50.131 50.895	1.00 0.00 1.00 0.00	B B
	MOTA	2131	HZ2 HZ3	LYS	174	19.398	74.161	50.926	1.00 0.00	В
	MOTA ATOM	2132 2133	nzз С	LYS	174 174	20.551 20.288	76.818	44.661	1.00 22.91	В
	ATOM	2133	0	LYS	174	20.420	77.948	45.110	1.00 22.73	В
10	ATOM	2135	И	ALA	175	21.279	76.173	44.059	1.00 23.45	B
10	ATOM	2136	H	ALA	175	21.134	75.270	43.705	1.00 0.00	В
	MOTA	2137	CA	ALA	175	22.589	76.807	43.929	1.00 26.35	В
	MOTA	2138	CB	ALA	175	23.694	75.755	43.981	1.00 22.79	В
	ATOM	2139	C	ALA	175	22.730	77.649	42.658	1.00 26.76	В
15	ATOM	2140	0	ALA	175	23.651	78.460	42.539	1.00 29.91	В
	MOTA	2141	N	MET	176	21.821	77.470	41.710	1.00 25.18	В
	MOTA	2142	H	MET	176	21.098	76.822	41.845	1.00 0.00	В
	MOTA	2143	CA	MET	176	21.888	78.226	40.467	1.00 24.53	В
20	MOTA	2144	CB	MET	176	21.253	77.418	39.336	1.00 22.97	В
20	ATOM	2145	CG	MET	176	21.779	76.003	39.265	1.00 22.20	В
	MOTA	2146	SD	MET	176	20.923	74.945	38.090	1.00 24.68 1.00 19.10	В В
	ATOM	2147	CE	$_{ m MET}$	176 176	22.0 <b>4</b> 5 21.227	73.494 79.595	38.136 40.548	1.00 19.10	В
	ATOM ATOM	2148 2149	C O	MET	176	20.618	79.958	41.554	1.00 24.31	В
25	ATOM	2150	N	ASP	177	21.365	80.354	39.469	1.00 24.61	В
23	ATOM	2151	H	ASP	177	21.887	80.004	38.717	1.00 0.00	В
	ATOM	2152	CA	ASP	$\frac{177}{177}$	20.777	81.678	39.355	1.00 24.49	В
	ATOM	2153	CB	ASP	177	21.848	82.729	39.075	1.00 30.14	В
	ATOM	2154	CG	ASP	177	21.348	84.131	39.296	1.00 33.29	В
30	MOTA	2155	OD1	ASP	177	22.134	84.977	39.767	1.00 37.03	В
	ATOM	2156	OD2		177	20.160	84.388	39.000	1.00 42.39	В
	ATOM	2157	C	ASP	177	19.881	81.525	38.153	1.00 21.41	В
	ATOM	2158	0	ASP	177	20.365	81.519	37.017	1.00 20.00	В
25	MOTA	2159	N	ILE	178	18.581	81.390	38.407 39.336	1.00 18.68 1.00 0.00	B B
35	MOTA	2160 2161	H CA	ILE	178 178	18.270 17.610	81.436 81.169	37.350	1.00 0.00	В
	ATOM ATOM	2162	CB	ILE	178	16.525	80.193	37.788	1.00 24.17	В
	ATOM	2163	CG2	ILE	178	15.745	79.714	36.559	1.00 26.64	В
	ATOM	2164	CG1	ILE	178	17.154	79.024	38.560	1.00 26.03	В
40	ATOM	2165	CD1	ILE	178	17.407	77.790	37.734	1.00 21.54	В
	ATOM	2166	C	ILE	178	16.916	82.410	36.840	1.00 21.48	В
	ATOM	2167	0	ILE	178	16.327	83.164	37.598	1.00 13.16	В
	ATOM	2168	N	GLY	179	16.977	82.586	35.527	1.00 23.27	В
. ~	MOTA	2169	H	GLY	179	17.457	81.937	34.974	1.00 0.00	В
45	ATOM	2170	CA	GLY	179	16.346	83.727	34.904	1.00 24.96 1.00 25.44	B B
	ATOM	2171	C	GLY	179 179	16.621 17.505	83.775 83.087	33.414 32.906	1.00 23.44	В
	ATOM	2172 2173	N	GLY PRO	180	15.844	84.583	32.685	1.00 10.00	В
	ATOM ATOM	2174	CD	PRO	180	14.721	85.395	33.194	1.00 27.30	В
50	ATOM	2175	CA	PRO	180	16.006	84.725	31.240	1.00 25.34	В
50	ATOM	2176	CB	PRO	180	14.991	85.817	30.881	1.00 28.96	В
	ATOM	2177	CG	PRO	180	13.934	85.689	31.956	1.00 21.85	В
	ATOM	2178	C	PRO	180	17.434	85.104	30.859	1.00 21.40	В
	MOTA	2179	0	PRO	180	17.889	84.771	29.780	1.00 17.19	В
55	MOTA	2180	N	LYS	181	18.126	85.779	31.773	1.00 22.62	В
	MOTA	2181	H	LYS	181	17.698	85.977	32.631	1.00 0.00	В
	MOTA	2182	CA	LYS	181	19.493	86.244	31.555	1.00 22.16	В
	MOTA	2183	CB	LYS	181	19.628	87.682	32.050	1.00 27.02	В
60	ATOM	2184	CG	LYS	181	18.711	88.652	31.352 29.925	1.00 32.06 1.00 29.94	B B
60	ATOM	2185	CD	LYS LYS	181 181	19.157 19.909	88.876 90.182	29.788	1.00 29.94	В
	ATOM ATOM	2186 2187	CE NZ	LYS	181	20.167	90.503	28.357	1.00 34.68	В
	ATOM	2188		LYS	181	19.264	90.584	27.850	1.00 0.00	В
	ATOM	2189		LYS	181	20.738	89.744	27.930	1.00 0.00	В
65	ATOM	2190		LYS	181	20.685	91.402	28.291	1.00 0.00	В
	ATOM	2191	C	LYS	181	20.585	85.395	32.206	1.00 22.21	В
	ATOM	2192	0	LYS	181	21.764	85.684	32.044	1.00 20.87	В
	MOTA	2193	N	GLN	182	20.194	84.379	32.958	1.00 23.88	В
	ATOM	2194	H	GLN	182	19.235	84.212	33.077	1.00 0.00	В
70	MOTA	2195	CA	GLN	182	21.156	83.498	33.616	1.00 27.46	В
	ATOM	2196	CB	GLN	182	21.004	83.585	35.136	1.00 31.07	В
	ATOM	2197	CG	GLN	182	20.735	84.991	35.668 35.421	1.00 38.02 1.00 42.63	В В
	MOTA	2198	$^{\rm CD}$	GLN	182	21.886	85.950	JJ.441	1.00 42.03	ם

NOME   2109   OE1 GLN   182   21.708   87.167   35.455   1.00   44.04   34.708   200   NE2 GLN   182   23.171   84.431   35.184   1.00   0.00   34.708   202   NE2 GLN   182   23.171   84.431   35.184   1.00   0.00   34.708   202   NE2 GLN   182   23.824   84.012   35.029   1.00   0.00   34.708   2204   OE GLN   182   20.886   82.076   33.135   1.00   22.08   24.00   24.											
Profession   Pro		АТОМ	2199	OE1	GLN	182	21.708	87.167	35,435	1.00 44.04	В
ATOM   2201   HE21 GIM   182   23.171   84.431   35.184   1.00   0.00   B											
ATOM   2202   EB22   CIAN   182   23,824   86,012   35,029   1,00   26,08   B   ATOM   2204   O   GIAN   182   20,806   81,835   31,135   1,00   26,08   B   ATOM   2205   N   THR   183   20,732   81,132   31,313   1,00   22,28   B   ATOM   2206   H   THR   183   20,732   81,132   31,08   1,00   18,41   B   ATOM   2207   CA   THR   183   20,439   79,778   31,313   31,00   21,94   B   ATOM   2208   CB   THR   183   20,439   79,778   31,313   31,00   21,94   B   ATOM   2209   CB   THR   183   20,239   77,844   51,211   1,00   36,22   B   ATOM   2211   CG2   THR   183   20,239   77,844   51,211   1,00   36,22   B   ATOM   2211   CG2   THR   183   20,239   77,844   51,211   1,00   36,22   B   ATOM   2211   CG2   THR   183   20,239   77,844   51,512   1,00   36,22   B   ATOM   2211   CG2   THR   183   20,238   77,402   34,488   1,00   0,00   0   B   ATOM   2211   CG2   THR   183   20,238   77,402   34,488   1,00   0,00   0   B   ATOM   2211   CG2   THR   183   18,681   77,402   34,488   1,00   0,00   0   B   ATOM   2211   CG2   THR   183   188   178   80,93   14,360   1,00   19,07   B   ATOM   2214   CG2   THR   183   188   178   80,93   14,360   1,00   19,07   B   ATOM   2214   CG2   THR   183   184   18,509   78,607   21,797   1,00   15,936   B   ATOM   2216   CG   GLN   184   17,107   78,245   22,259   1,00   0,00   B   ATOM   2217   CB   GLN   184   16,564   78,600   31,305   1,00   10,017   B   ATOM   2220   CB   GLN   184   16,243   80,079   31,118   1,00   15,38   B   ATOM   2221   CD   GLN   184   16,243   80,079   31,118   1,00   15,38   B   ATOM   2221   CD   GLN   184   16,243   80,079   31,188   1,00   10,017   18   ATOM   2222   CD   GLN   184   14,165   78,901   28,859   1,00   17,14   B   ATOM   2222   CD   GLN   184   14,165   78,901   28,859   1,00   17,14   B   ATOM   2222   CD   GLN   184   14,165   78,901   28,859   1,00   17,14   B   ATOM   2222   CD   GLN   184   14,165   78,901   28,859   1,00   17,14   B   ATOM   2222   CD   GLN   184   14,165   78,901   28,859   1,00   17,14   B   ATOM   22											В
5 AROM 2203 C GIAN 182 20.880 82.076 33.135 1.00 26.08 B AROM 2205 N THR 183 20.823 81.355 31.926 1.00 22.28 B AROM 2205 N THR 183 20.823 81.355 31.926 1.00 22.28 B AROM 2205 N THR 183 20.823 81.355 31.926 1.00 22.28 B AROM 2207 CA THR 183 20.823 81.355 31.926 1.00 18.41 B AROM 2207 CA THR 183 20.823 81.355 31.00 1.00 21.00 0.00 B AROM 2207 CA THR 183 20.823 81.355 31.00 1.00 27.45 B AROM 2209 CGI THR 183 20.823 81.355 31.00 1.00 27.45 B AROM 2209 CGI THR 183 21.165 78.705 34.513 1.00 27.45 B AROM 2210 HGI THR 183 19.691 77.402 34.438 1.00 0.00 36.22 B AROM 2211 CG2 THR 183 19.691 77.402 34.438 1.00 0.00 B AROM 2211 CG2 THR 183 19.691 77.402 34.438 1.00 10.00 18.10 B AROM 2211 CG2 THR 183 18.958 79.531 36.646 1.00 18.10 18.10 B AROM 2215 CG THR 183 18.958 79.531 34.560 1.00 10.00 18.10 B AROM 2215 CG GIAN 184 18.558 79.561 36.646 1.00 10.00 18.10 B AROM 2215 CG GIAN 184 18.558 79.513 34.360 1.00 10.00 10.96 B AROM 2215 CG GIAN 184 17.107 78.245 52.693 1.00 10.96 B AROM 2215 CG GIAN 184 16.564 78.600 13.005 1.00 10.00 10.96 B AROM 2219 CD GIAN 184 16.546 78.600 31.005 10.00 10.00 18. B AROM 2219 CD GIAN 184 15.181 80.307 31.118 1.00 10.03 18 B AROM 2219 CD GIAN 184 15.181 80.307 30.063 1.00 10.14.63 B AROM 2219 CD GIAN 184 15.181 80.307 30.063 1.00 10.14.63 B AROM 2221 NEZ GIAN 184 15.181 80.307 30.063 1.00 10.14.69 B AROM 2222 HEZ1 GIAN 184 17.107 78.245 21.225 10.00 10.46.63 B AROM 2222 CG GIAN 184 17.107 78.245 21.225 10.00 10.46.63 B AROM 2222 CG GIAN 184 17.107 78.245 21.225 10.00 10.46.63 B AROM 2223 CG GIAN 184 17.107 78.245 21.225 10.00 10.00 B AROM 2223 CG GIAN 184 17.107 78.245 21.225 10.00 10.00 B AROM 2223 CG GIAN 184 17.107 78.245 21.225 10.00 10.00 B AROM 2223 CG GIAN 184 17.023 76.740 32.905 1.00 10.00 18.05 B AROM 2223 CG GIAN 184 17.023 76.740 32.905 1.00 10.00 18.05 B AROM 2223 CG GIAN 184 17.023 76.740 32.905 1.00 10.00 18.05 B AROM 2223 CG GIAN 184 17.947 79.942 23.277 1.00 10.00 18.55 B AROM 2223 CG GIAN 184 17.947 79.942 23.377 1.00 10.00 18.55 B AROM 2223 CG GIAN 186 17.107 186 187 79.942											
AROM 2204 C GLN 182 20.806 81.835 31.926 1.00 22.28 B AROM 2205 N THR 183 20.732 81.132 41.058 1.00 18.41 B AROM 2206 C THR 183 20.732 81.132 41.058 1.00 10.00 B AROM 2207 CA THR 183 20.439 79.778 31.640 1.00 21.94 B AROM 2208 CS THR 183 20.439 79.778 31.640 1.00 21.94 B AROM 2209 CS THR 183 20.203 77.344 31.60 1.00 27.45 B AROM 2210 CS THR 183 20.203 77.344 31.00 27.45 B AROM 2210 HS1 THR 183 120.203 77.344 31.00 27.45 B AROM 2211 CS THR 183 20.203 77.344 31.00 27.45 B AROM 2211 CS THR 183 20.203 77.344 31.00 0.00 B AROM 2211 C THR 183 19.691 77.002 34.488 1.00 0.00 D B AROM 2212 C THR 183 20.203 77.344 31.00 10.00 10.00 B AROM 2212 C THR 183 20.203 77.344 31.00 10.00 10.00 B AROM 2214 N GLN 184 18.509 78.607 21.2797 1.00 15.96 B AROM 2214 N GLN 184 18.509 78.607 22.797 1.00 15.96 B AROM 2215 C GLN 184 18.139 78.600 31.305 1.00 19.07 B AROM 2215 C GLN 184 17.107 78.245 22.693 1.00 0.00 B AROM 2217 CB GLN 184 16.564 78.600 31.305 1.00 15.38 B AROM 2219 CD GLN 184 16.564 78.600 31.305 1.00 15.38 B AROM 2220 CB GLN 184 16.564 78.600 31.305 1.00 15.38 B AROM 2221 NEZ GLN 184 14.165 80.926 30.326 1.00 17.14 B AROM 2221 NEZ GLN 184 14.165 80.926 30.326 1.00 17.14 B AROM 2222 HEZZ GLN 184 14.167 79.801 28.859 1.00 17.14 B AROM 2222 HEZZ GLN 184 14.167 79.801 28.859 1.00 17.14 B AROM 2222 HEZZ GLN 184 14.167 79.801 28.859 1.00 17.14 B AROM 2222 HEZZ GLN 184 14.167 79.801 28.859 1.00 17.14 B AROM 2222 HEZZ GLN 184 14.167 79.801 28.859 1.00 17.14 B AROM 2222 HEZZ GLN 184 14.167 79.801 28.859 1.00 17.14 B AROM 2222 C CLN 185 15.467 79.305 28.6594 1.00 10.00 B AROM 2222 C C VAL 185 15.467 79.305 28.6594 1.00 10.00 B AROM 2223 C VAL 185 15.467 79.305 28.6594 1.00 10.00 B AROM 2223 C VAL 185 15.467 79.305 28.6594 1.00 10.00 15.58 B AROM 2223 C VAL 185 15.467 79.305 28.6594 1.00 10.00 15.58 B AROM 2223 C VAL 185 15.467 79.305 29.505 1.00 14.59 B AROM 2223 C VAL 185 15.467 79.305 29.505 1.00 14.59 B AROM 2223 C VAL 185 15.467 79.305 29.505 1.00 14.59 B AROM 2223 C VAL 185 11.85 11.305 79.305 29.505 1.00 14.59 B AROM 2235 C VA	5									1.00 26.08	В
APOM   2206   H   THE   183   20.823   81.550   55.010   1.00   0.00   B	•								31.926	1.00 22.28	В
ACCM  2207 CA   THE   193   20.439   79.778   33.640   1.00   21.94   B   ACCM  2209   CG1   THR   183   20.203   77.844   35.121   1.00   36.22   B   ACCM  2210   CG2   THR   183   20.203   77.844   35.121   1.00   36.22   B   ACCM  2211   CG2   THR   183   20.203   77.844   35.121   1.00   36.22   B   ACCM  2211   CG2   THR   183   20.208   79.347   35.563   1.00   20.20   B   ACCM  2212   C   THR   183   18.978   79.531   33.646   1.00   10.01   B   ACCM  2213   O   THR   183   18.978   79.531   33.646   1.00   18.10   B   ACCM  2214   N   GLN   184   18.509   78.607   32.797   1.00   15.96   B   ACCM  2215   H   GLN   184   18.509   78.607   32.797   1.00   15.96   B   ACCM  2216   CA   GLN   184   17.107   76.245   32.693   1.00   10.01   0.70   B   ACCM  2217   CB   GLN   184   17.107   76.245   32.693   1.00   10.73   B   ACCM  2219   CD   GLN   184   16.564   78.600   31.305   1.00   10.17   B   ACCM  2219   CD   GLN   184   15.181   80.307   30.326   1.00   14.63   B   ACCM  2220   MEZ   GLN   184   15.181   80.307   30.326   1.00   17.84   B   ACCM  2221   MEZ   GLN   184   15.416   79.801   28.859   1.00   17.84   B   ACCM  2222   MEZ   GLN   184   15.416   79.801   28.859   1.00   10.78   B   ACCM  2223   MEZ   GLN   184   16.245   79.305   28.694   1.00   10.00   B   ACCM  2224   MEZ   GLN   184   17.841   75.981   32.377   1.00   16.49   B   ACCM  2224   CG   GLN   184   17.841   75.981   32.377   1.00   16.49   B   ACCM  2224   CG   GLN   184   17.841   75.981   32.377   1.00   16.49   B   ACCM  2225   CG   GLN   184   17.841   75.981   32.377   1.00   16.49   B   ACCM  2225   CG   GLN   184   17.841   75.981   32.377   1.00   16.49   B   ACCM  2225   CG   GLN   185   16.495   76.381   33.945   1.00   10.00   B   ACCM  2225   CG   GLN   185   16.495   76.892   33.946   1.00   10.00   B   ACCM  2226   CG   VAL   185   16.495   76.892   33.945   1.00   10.00   B   ACCM  2226   CG   VAL   185   16.495   76.892   33.946   1.00   10.00   B   ACCM  2226   CG   VAL   185   16.495   76.893   33.946   1				N		183	20.732	81.132	34.058	1.00 18.41	В
10		ATOM	2206	H	THR	183	20.823	81.350	35.010	1.00 0.00	В
ATOM 2209 GSI THR 183		MOTA	2207	CA	THR	183	20.439	79.778	33.640	1.00 21.94	В
ATOM 2210 BGI THR 183 19.691 77.402 34.438 1.00 0.00 B ATOM 2211 C C THR 183 22.028 79.347 35.563 1.00 20.20 B ATOM 2212 C THR 183 18.936 79.531 33.646 1.00 18.10 B ATOM 2213 O THR 183 18.936 79.531 33.4360 1.00 19.07 B ATOM 2214 N GIN 184 18.509 78.607 32.797 1.00 15.96 B ATOM 2215 C G GIN 184 19.157 78.1645 32.255 1.00 0.00 B ATOM 2216 CA GIN 184 19.157 78.1645 32.255 1.00 0.00 B ATOM 2217 CB GIN 184 17.107 78.245 32.693 1.00 16.73 B ATOM 2217 CB GIN 184 16.243 80.079 31.118 1.00 15.38 B ATOM 2219 CD GIN 184 15.181 80.307 31.063 1.00 14.63 B ATOM 2219 CD GIN 184 15.181 80.307 31.063 1.00 14.63 B ATOM 2221 NEZ GIN 184 15.181 80.307 30.063 1.00 16.73 B ATOM 2222 HEZ1 GIN 184 15.181 80.307 30.063 1.00 16.73 B ATOM 2222 HEZ2 GIN 184 15.416 79.801 28.859 1.00 17.14 B ATOM 2223 HEZ2 GIN 184 15.417 79.942 28.172 1.00 0.00 B ATOM 2224 C G GIN 184 17.023 76.740 32.905 1.00 16.49 B ATOM 2225 C G GIN 184 17.023 76.740 32.905 1.00 16.49 B ATOM 2226 N VALI 185 15.437 76.962 34.095 1.00 18.49 B ATOM 2227 H VAL 185 15.437 76.962 34.095 1.00 18.64 B ATOM 2229 C VAL 185 15.849 74.895 33.943 1.00 15.68 B ATOM 2229 C VAL 185 15.608 73.149 35.795 1.00 16.93 B ATOM 2233 C VAL 185 15.608 73.149 35.795 1.00 16.99 B ATOM 2233 C VAL 185 15.608 73.149 35.795 1.00 16.99 B ATOM 2233 C VAL 185 15.437 76.962 33.995 1.00 17.38 B ATOM 2233 C VAL 185 15.437 76.962 33.993 1.00 17.38 B ATOM 2233 C VAL 185 16.145 74.549 33.933 1.00 17.38 B ATOM 2234 N GLY 186 13.104 74.596 33.3923 1.00 10.78 B ATOM 2235 C VAL 185 17.641 74.506 33.541 1.00 10.74 B ATOM 2235 C VAL 185 17.641 74.506 33.3923 1.00 10.78 B ATOM 2236 C A GLY 186 13.104 74.596 33.3933 1.00 10.78 B ATOM 2237 C GLY 186 13.104 74.596 33.3933 1.00 10.78 B ATOM 2233 C GLY 186 13.104 74.596 33.3933 1.00 10.78 B ATOM 2235 C GLY 186 13.104 74.596 33.3933 1.00 10.78 B ATOM 2235 C GLY 186 13.104 74.596 33.3931 1.00 10.78 B ATOM 2236 C GLY 188 11.79 6.963 33.903 1.00 10.78 B ATOM 2237 C GLY 188 11.79 6.963 33.903 1.00 10.78 B ATOM 2238 C G VAL 185 17.647 74.596 33.393 31.00 10.00 B ATOM 2237 C G	10	ATOM	2208	CB	THR	183	21.165		34.513	1.00 27.45	В
MICON   2211   CG2 THR   183   22.028   79.347   35.563   1.00   20.20   B		ATOM	2209	0G1	THR	183	20.203	77.844	35.121	1.00 36.22	В
ATOM   2212   C		MOTA	2210	HG1	THR	183	19.691	77.402			
15		MOTA	2211	CG2		183					
ATOM   2214   N   GLN   184   18.509   78.607   32.797   1.00   15.96   B   ATOM   2215   CA   GLN   184   19.158   78.154   32.225   1.00   0.00   B   ATOM   2217   CB   GLN   184   17.107   78.245   32.693   1.00   16.73   B   ATOM   2218   CG   GLN   184   16.243   80.079   31.118   1.00   15.38   B   ATOM   2219   CG   GLN   184   16.243   80.079   31.118   1.00   15.38   B   ATOM   2220   OEL   GLN   184   14.165   80.926   30.326   1.00   17.14   B   ATOM   2221   HEZ   GLN   184   14.165   80.926   30.326   1.00   17.14   B   ATOM   2222   HEZ   GLN   184   16.245   79.305   28.694   1.00   0.01   17.84   B   ATOM   2222   HEZ   GLN   184   16.245   79.305   28.694   1.00   0.00   0.00   B   ATOM   2224   CC   GLN   184   16.245   79.305   28.694   1.00   0.00   0.00   B   ATOM   2224   CC   GLN   184   17.023   76.740   32.905   1.00   16.49   ATOM   2222   GLN   184   17.023   76.740   32.905   1.00   16.49   ATOM   2222   CC   VAL   185   16.043   76.311   33.685   1.00   19.05   B   ATOM   2228   CC   VAL   185   15.437   76.942   34.197   1.00   18.75   B   ATOM   2229   CR   VAL   185   15.437   76.943   33.943   1.00   15.68   B   ATOM   2229   CR   VAL   185   15.608   73.149   35.795   1.00   14.91   B   ATOM   2223   CR   VAL   185   15.608   73.149   35.795   1.00   14.91   B   ATOM   2223   CR   VAL   185   15.608   73.149   35.795   1.00   14.91   B   ATOM   2231   CG   VAL   185   15.608   73.149   35.795   1.00   14.91   B   ATOM   2231   CG   VAL   185   15.608   73.149   35.795   1.00   14.91   B   ATOM   2231   CG   VAL   185   15.608   73.149   35.795   1.00   14.91   B   ATOM   2231   CG   VAL   185   15.608   73.149   35.795   1.00   14.91   B   ATOM   2234   N   GLY   186   13.145   71.359   33.668   1.00   10.774   B   ATOM   2234   N   GLY   186   13.145   71.359   33.668   1.00   10.774   B   ATOM   2234   N   GLY   186   13.145   71.359   33.668   1.00   10.778   B   ATOM   2234   CR   GLY   186   13.145   71.359   33.666   1.00   10.778   B   ATOM   2235   CG   VAL   188   13		MOTA	2212	С	THR						
ATOM 2215 H GLN 184 19.158 78.154 32.225 1.00 0.00 0.00 ATOM 2217 CB GLN 184 16.564 78.600 31.305 1.00 16.73 B ATOM 2219 CD GLN 184 16.564 78.600 31.305 1.00 20.17 B ATOM 2219 CD GLN 184 16.243 80.007 30.163 1.00 14.63 B ATOM 2220 CBL GLN 184 15.181 80.307 30.063 1.00 14.63 B ATOM 2221 NB2 GLN 184 15.181 80.307 30.063 1.00 14.63 B ATOM 2221 NB2 GLN 184 15.181 80.307 30.063 1.00 14.63 B ATOM 2221 NB2 GLN 184 15.181 80.307 30.063 1.00 14.63 B ATOM 2222 HB21 GLN 184 15.416 79.801 28.859 1.00 17.84 B ATOM 2222 HB21 GLN 184 15.416 79.801 28.859 1.00 17.84 B ATOM 2223 NB22 GLN 184 14.737 79.942 28.172 1.00 0.00 B ATOM 2223 NB22 GLN 184 14.737 79.942 28.172 1.00 0.00 B ATOM 2225 CO GLN 184 17.841 75.981 32.377 1.00 18.75 B ATOM 2226 N VAL 185 16.043 76.311 33.685 1.00 10.00 B ATOM 2228 CA VAL 185 15.849 74.895 33.943 1.00 15.68 B ATOM 2220 CGV VAL 185 15.608 73.149 35.795 1.00 15.74 B ATOM 2220 CGV VAL 185 15.608 73.149 35.795 1.00 13.27 B ATOM 2231 CGV VAL 185 15.608 73.149 35.795 1.00 14.91 B ATOM 2231 CGV VAL 185 15.608 73.149 35.795 1.00 14.91 B ATOM 2231 CGV VAL 185 15.608 73.149 35.795 1.00 14.91 B ATOM 2231 CGV VAL 185 15.608 73.343 35.795 1.00 13.27 B ATOM 2232 CV VAL 185 15.608 73.346 32.948 1.00 12.73 B ATOM 2231 CGV VAL 185 15.608 73.346 32.948 1.00 12.73 B ATOM 2231 CGV VAL 185 15.407 74.895 33.943 1.00 17.38 B ATOM 2231 CGV VAL 186 13.147 74.506 33.614 1.00 16.98 B ATOM 2231 CGV VAL 186 13.147 74.506 33.614 1.00 16.98 B ATOM 2231 CGV VAL 186 13.147 74.506 33.614 1.00 16.98 B ATOM 2231 CGV VAL 186 13.147 74.506 33.614 1.00 16.98 B ATOM 2234 CGV LLE 187 11.152 77.172 33.469 1.00 17.78 B ATOM 2235 CGV LLE 187 11.152 77.172 33.346 1.00 17.78 B ATOM 2234 CGV LLE 187 11.152 77.172 33.346 1.00 17.78 B ATOM 2244 CGV LLE 187 11.152 77.172 33.346 1.00 17.78 B ATOM 2245 CGV LLE 187 11.152 77.172 33.346 1.00 17.78 B ATOM 2246 CGV LLE 187 11.152 77.172 33.346 1.00 17.78 B ATOM 2245 CGV LLE 187 11.152 77.172 33.346 1.00 17.78 B ATOM 2245 CGV LLE 187 11.152 77.172 33.346 1.00 17.78 B ATOM 2255 CGV LLE 187 11.152 77.77 6	15	MOTA		0							
ATOM   2216   CA   GLN   184   17.107   78.245   32.693   1.00   16.73   B   ATOM   2217   CB   GLN   184   16.564   78.600   31.305   1.00   20.17   B   ATOM   2218   CG   GLN   184   16.243   80.079   31.118   1.00   15.38   B   ATOM   2220   OEI   GLN   184   14.165   80.926   30.326   1.00   14.63   B   ATOM   2221   NEZ   GLN   184   14.165   80.926   30.326   1.00   17.14   B   ATOM   2221   NEZ   GLN   184   14.165   80.926   30.326   1.00   17.14   B   ATOM   2221   NEZ   GLN   184   16.245   79.305   28.694   1.00   0.00   0.00   B   ATOM   2224   CE   GLN   184   16.245   79.305   28.694   1.00   0.00   0.00   B   ATOM   2224   CG   GLN   184   17.023   76.740   32.905   1.00   16.49   B   ATOM   2224   CG   GLN   184   17.023   76.740   32.905   1.00   16.49   B   ATOM   2225   NAL   185   16.043   76.311   33.685   1.00   19.05   B   ATOM   2228   CD   VAL   185   16.043   76.311   33.685   1.00   19.05   B   ATOM   2228   CD   VAL   185   15.849   74.895   33.943   1.00   15.68   B   ATOM   2229   CD   VAL   185   15.608   73.149   35.795   1.00   10.491   B   ATOM   2223   CD   VAL   185   15.608   73.149   35.795   1.00   14.91   B   ATOM   2232   CD   VAL   185   15.608   73.149   35.795   1.00   14.91   B   ATOM   2232   CD   VAL   185   15.608   73.149   35.795   1.00   14.91   B   ATOM   2232   CD   VAL   185   15.608   73.149   35.795   1.00   14.91   B   ATOM   2232   CD   VAL   185   15.608   73.149   35.795   1.00   14.91   B   ATOM   2232   CD   VAL   185   15.608   73.364   32.948   1.00   17.38   B   ATOM   2232   CD   VAL   185   15.608   73.149   35.795   1.00   14.91   B   ATOM   2232   CD   VAL   185   15.608   73.364   32.948   1.00   17.38   B   ATOM   2232   CD   VAL   185   14.411   74.506   33.644   1.00   16.98   B   ATOM   2234   N   GLY   186   14.296   73.364   32.948   1.00   10.72   B   ATOM   2234   N   GLY   186   14.296   73.364   32.948   1.00   10.74   B   ATOM   2234   CD   14.88   14.897   14.509   14.599   14.599   14.599   14.599   14.599   14.599   14.599   1		ATOM									
ATOM   2217   CB   GLN   184											
ATOM											
ATOM   2219   CD   GLN   184	20										
ATOM	20										
ATOM   2221 NBC   CIN   184											
ATOM   2222   HE21   GLN   184   16.245   79.305   28.694   1.00   0.00   B											
25 ATOM 2223 HE22 CLN 184 14.737 79.942 28.172 1.00 0.00 B ATOM 2224 C GLN 184 17.023 76.740 32.905 1.00 16.49 B ATOM 2225 O GLN 184 17.023 76.740 32.905 1.00 16.49 B ATOM 2226 N VAL 185 16.043 76.311 33.685 1.00 19.05 B ATOM 2227 H VAL 185 15.437 76.962 34.095 1.00 0.00 B ATOM 2228 CA VAL 185 15.437 76.962 34.095 1.00 0.00 B ATOM 2229 CB VAL 185 15.437 76.962 34.095 1.00 15.74 B ATOM 2220 CG VAL 185 15.437 74.549 35.437 1.00 15.74 B ATOM 2230 CG1 VAL 185 15.608 73.149 35.795 1.00 14.91 B ATOM 2231 CG2 VAL 185 17.641 74.540 35.686 1.00 13.27 B ATOM 2231 CG VAL 185 14.411 74.506 33.644 1.00 16.98 B ATOM 2231 C VAL 185 14.411 74.506 33.644 1.00 16.98 B ATOM 2235 H GLY 186 14.296 73.364 32.948 1.00 20.72 B ATOM 2235 H GLY 186 15.109 72.886 32.688 1.00 0.00 B ATOM 2237 C GLY 186 13.016 72.794 32.585 1.00 14.37 B ATOM 2239 N ILE 187 12.020 70.721 33.409 1.00 17.74 B ATOM 2239 N ILE 187 12.020 70.721 33.409 1.00 10.74 B ATOM 2241 CA ILE 187 11.152 71.722 33.409 1.00 10.74 B ATOM 2241 CA ILE 187 11.152 71.722 33.409 1.00 10.78 B ATOM 2242 CB ILE 187 11.766 69.193 35.366 1.00 0.00 B ATOM 2243 CG2 ILE 187 11.766 69.193 35.366 1.00 0.00 B ATOM 2244 CG1 ILE 187 12.04 69.344 33.869 1.00 10.78 B ATOM 2242 CB ILE 187 11.766 69.193 35.366 1.00 0.00 B ATOM 2242 CB ILE 187 11.766 69.193 35.366 1.00 0.00 B ATOM 2242 CB ILE 187 11.766 69.993 35.366 1.00 0.00 B ATOM 2242 CB ILE 187 11.766 69.193 35.366 1.00 0.00 B ATOM 2242 CB ILE 187 11.766 69.193 35.366 1.00 0.00 14.75 B ATOM 2242 CB ILE 187 11.766 69.193 35.366 1.00 0.00 14.75 B ATOM 2242 CB ILE 187 11.796 69.193 35.762 1.00 10.78 B ATOM 2242 CB ILE 187 11.796 69.193 35.366 1.00 0.00 14.75 B ATOM 2242 CB ILE 187 11.796 69.193 35.366 1.00 0.00 14.75 B ATOM 2245 CDI ILE 187 12.517 69.886 37.678 1.00 10.00 15.84 B ATOM 2245 CDI ILE 187 12.517 69.886 37.678 1.00 10.00 15.80 B ATOM 2246 C ILE 187 11.791 68.422 33.105 1.00 10.00 15.80 B ATOM 2248 N VAL 188 11.746 66.277 31.970 1.00 16.65 B ATOM 2248 N VAL 188 11.746 66.277 31.970 1.00 16.65 B ATOM 2248 C VAL 188 11.89 9.094 64.60 33.											
ATOM 22224 C GIN 184 17.023 76.740 32.905 1.00 16.49 B ATOM 2225 O GIN 184 17.841 75.981 32.377 1.00 18.75 B ATOM 2226 N VAL 185 16.043 76.311 33.685 1.00 19.05 B ATOM 2227 H VAL 185 15.437 76.962 34.095 1.00 0.00 B ATOM 2229 CB VAL 185 15.437 76.962 34.095 1.00 19.06 B ATOM 2229 CB VAL 185 15.608 74.593 33.943 1.00 15.68 B ATOM 2229 CC VAL 185 15.608 74.593 33.943 1.00 15.68 B ATOM 2231 CC2 VAL 185 15.608 74.549 35.437 1.00 15.74 B ATOM 2231 CC2 VAL 185 17.641 74.610 35.686 1.00 14.91 B ATOM 2232 C VAL 185 17.641 74.610 35.686 1.00 10.74 B ATOM 2233 N CAL 185 13.458 75.230 33.923 1.00 16.98 B ATOM 2233 N GLY 186 15.109 72.886 32.688 1.00 0.00 B ATOM 2237 C GLY 186 15.109 72.886 32.688 1.00 0.00 B ATOM 2238 N GLY 186 13.134 71.359 33.073 1.00 16.88 B ATOM 2238 N GLY 186 13.134 71.359 33.073 1.00 16.88 B ATOM 2239 N LLE 187 12.020 70.225 33.165 1.00 10.74 B ATOM 2239 N LLE 187 12.020 70.221 33.409 1.00 12.53 B ATOM 2240 H LLE 187 11.152 71.172 33.346 1.00 10.74 B ATOM 2240 CB LLE 187 11.756 69.193 35.366 1.00 10.75 B ATOM 2241 CB LLE 187 11.736 69.193 35.366 1.00 10.75 B ATOM 2242 CB LLE 187 11.736 69.193 35.366 1.00 10.75 B ATOM 2244 CGI LLE 187 11.736 69.193 35.366 1.00 10.75 B ATOM 2248 N VAL 188 11.756 69.193 35.366 1.00 14.75 B ATOM 2248 N VAL 188 11.756 69.193 35.366 1.00 14.75 B ATOM 2248 N VAL 188 11.756 69.293 32.698 1.00 14.75 B ATOM 2248 N VAL 188 11.756 67.299 32.696 1.00 10.78 B ATOM 2248 N VAL 188 11.756 67.299 32.696 1.00 10.78 B ATOM 2248 N VAL 188 11.756 67.299 32.696 1.00 10.79 B ATOM 2249 N VAL 188 11.756 67.299 32.696 1.00 10.79 B ATOM 2245 CD VAL 188 11.756 67.299 32.696 1.00 10.79 B ATOM 2245 CD VAL 188 11.756 67.299 32.696 1.00 10.79 B ATOM 2245 CD VAL 188 11.756 67.299 32.696 1.00 10.79 B ATOM 2245 CD VAL 188 11.756 67.299 32.696 1.00 10.79 B ATOM 2255 CG VAL 188 11.756 67.299 32.696 1.00 10.79 B ATOM 2255 CG VAL 188 11.756 67.299 32.696 1.00 10.79 B ATOM 2255 CG VAL 188 11.756 67.299 32.696 1.00 10.79 B ATOM 2255 CG VAL 188 11.756 67.299 32.897 1.00 10.00 B ATOM 2255 HEZ CLIN 189 9.993 6	25										
ATOM	23										
ATOM   2227   N   VAL   185   16.043   76.311   33.685   1.00   19.05   B											
ATOM   2228   CA   VAL   185   15.437   76.962   34.095   1.00   0.00   B   ATOM   2229   CB   VAL   185   15.849   74.8495   33.943   1.00   15.68   B   ATOM   2229   CB   VAL   185   16.145   74.549   35.437   1.00   15.74   B   ATOM   2230   CG1   VAL   185   15.608   73.149   35.795   1.00   14.91   B   ATOM   2231   CC2   VAL   185   17.641   74.610   35.686   1.00   13.27   B   ATOM   2232   C   VAL   185   14.411   74.506   33.614   1.00   16.98   B   ATOM   2234   N   GLY   186   14.296   73.364   32.948   1.00   20.72   B   ATOM   2235   CA   GLY   186   14.296   73.364   32.948   1.00   20.72   B   ATOM   2236   CA   GLY   186   13.016   72.794   32.585   1.00   14.37   B   ATOM   2236   CA   GLY   186   13.016   72.794   32.585   1.00   14.37   B   ATOM   2237   C   GLY   186   13.134   71.359   33.073   1.00   16.88   B   ATOM   2239   N   LLE   187   11.152   71.172   33.409   1.00   10.74   B   ATOM   2240   H   LLE   187   11.152   71.172   33.409   1.00   12.53   B   ATOM   2241   CA   LLE   187   11.152   71.172   33.409   1.00   14.75   B   ATOM   2241   CA   LLE   187   11.152   71.172   33.346   1.00   0.00   B   ATOM   2242   CB   LLE   187   11.736   69.143   35.742   1.00   10.78   B   ATOM   2244   CG1   LLE   187   11.736   69.913   35.566   1.00   9.81   B   ATOM   2245   CD1   LLE   187   11.33   67.712   35.742   1.00   10.78   B   ATOM   2245   CD1   LLE   187   11.33   67.712   35.742   1.00   10.78   B   ATOM   2245   CD1   LLE   187   11.36   66.99   32.908   1.00   14.75   B   ATOM   2245   CD1   LLE   187   11.39   68.422   33.105   1.00   12.90   B   ATOM   2245   CD1   LLE   187   11.39   69.901   36.207   1.00   10.78   B   ATOM   2245   CD1   LLE   187   11.39   69.901   36.207   1.00   10.78   B   ATOM   2245   CD1   LLE   187   11.39   69.901   36.207   1.00   10.78   B   ATOM   2245   CD1   LLE   187   11.36   66.999   32.908   1.00   14.75   B   ATOM   2250   CA   VAL   188   11.366   67.299   32.696   1.00   20.73   B   ATOM   2250   CA   VAL   188   11.366   67.299											
30											
ATOM   2229   CB   VAL   185   16.145   74.549   35.437   1.00   15.74   B   ATOM   2231   CG2   VAL   185   15.608   73.149   35.795   1.00   14.91   B   B   ATOM   2231   CG2   VAL   185   17.641   74.610   35.686   1.00   13.27   B   ATOM   2233   C   VAL   185   14.411   74.506   33.686   1.00   13.27   B   ATOM   2233   O   VAL   185   14.411   74.506   33.643   1.00   17.38   B   ATOM   2234   N   GLY   186   14.296   73.364   32.948   1.00   20.72   B   ATOM   2235   H   GLY   186   15.109   72.886   32.688   1.00   0.00   B   ATOM   2237   C   GLY   186   13.016   72.794   32.585   1.00   14.37   B   ATOM   2238   O   GLY   186   14.252   70.825   33.165   1.00   10.74   B   ATOM   2238   O   GLY   186   14.252   70.825   33.165   1.00   10.74   B   ATOM   2239   N   LLE   187   12.020   70.721   33.409   1.00   10.74   B   ATOM   2240   H   LLE   187   12.020   70.721   33.409   1.00   12.53   B   ATOM   2241   CA   LLE   187   11.766   69.344   33.869   1.00   14.75   B   ATOM   2242   CB   LLE   187   11.766   69.913   35.366   1.00   10.78   B   ATOM   2244   CGI   LLE   187   11.766   69.913   35.366   1.00   10.78   B   ATOM   2245   CDI   LLE   187   11.766   69.901   36.207   1.00   10.95   B   ATOM   2245   CDI   LLE   187   11.753   67.712   35.742   1.00   10.78   B   ATOM   2246   CDI   LLE   187   11.791   68.422   33.105   1.00   10.78   B   ATOM   2247   CDI   LLE   187   11.791   68.422   33.105   1.00   10.78   B   ATOM   2247   CDI   LLE   187   11.91   68.422   33.105   1.00   10.78   B   ATOM   2245   CDI   LLE   187   11.91   68.422   33.105   1.00   10.78   B   ATOM   2245   CDI   LLE   187   11.91   68.422   33.105   1.00   10.95   B   ATOM   2245   CDI   LLE   187   11.91   68.422   33.105   1.00   10.95   B   ATOM   2256   CA   VAL   188   11.748   65.977   30.620   1.00   20.73   B   ATOM   2255   CB   VAL   188   11.748   65.977   30.620   1.00   20.73   B   ATOM   2255   CB   VAL   188   11.432   67.075   29.602   1.00   16.65   B   ATOM   2255   CB   GLN   189   9.939   63	30										
ATOM   2231   CG2   VAL   185   15.608   73.149   35.795   1.00   14.91   B   ATOM   2232   C   VAL   185   17.641   74.506   33.614   1.00   13.27   B   B   ATOM   2232   C   VAL   185   14.411   74.506   33.614   1.00   15.98   B   ATOM   2234   N   GLY   186   14.296   73.364   32.948   1.00   20.72   B   ATOM   2235   H   GLY   186   14.296   73.364   32.948   1.00   20.72   B   ATOM   2237   C   GLY   186   13.016   72.794   32.585   1.00   14.37   B   ATOM   2237   C   GLY   186   13.134   71.359   33.073   1.00   14.37   B   ATOM   2238   N   GLY   186   13.134   71.359   33.073   1.00   16.88   B   ATOM   2239   N   LLE   187   11.152   71.172   33.466   1.00   0.00   B   ATOM   2240   H   LLE   187   11.152   71.172   33.366   1.00   0.00   B   ATOM   2241   CA   LLE   187   11.152   71.172   33.366   1.00   0.00   B   ATOM   2242   CB   LLE   187   11.733   67.712   33.366   1.00   0.00   B   ATOM   2242   CB   LLE   187   11.733   67.712   33.366   1.00   0.00   B   ATOM   2242   CG   LLE   187   11.733   67.712   33.366   1.00   0.00   B   ATOM   2242   CG   LLE   187   11.733   67.712   33.366   1.00   0.00   B   ATOM   2242   CG   LLE   187   11.733   67.712   33.366   1.00   0.00   B   ATOM   2243   CG2   LLE   187   11.733   67.712   33.366   1.00   0.076   B   ATOM   2245   CD1   LLE   187   12.517   69.886   37.678   1.00   10.78   B   ATOM   2246   C   LLE   187   12.517   69.886   37.678   1.00   7.68   B   ATOM   2247   O   LLE   187   11.914   68.422   33.105   1.00   10.78   B   ATOM   2248   N   VAL   188   11.756   67.299   32.996   1.00   20.73   B   ATOM   2250   CA   VAL   188   11.756   67.299   32.996   1.00   20.73   B   ATOM   2250   CG   VAL   188   11.748   65.977   30.620   1.00   31.42   B   ATOM   2255   CG   VAL   188   11.363   64.610   30.107   1.00   12.90   B   ATOM   2255   CG   CM   Lass   11.432   67.075   29.892   20.811   1.00   20.75   B   ATOM   2255   CG   CM   189   9.938   63.076   33.742   1.00   10.65   B   ATOM   2256   CG   CM   189   9.938   63.076   33											В
ATOM   2232   C   VAL   185   14.411   74.506   33.614   1.00   16.98   B   ATOM   2234   N   GLY   186   14.296   73.364   32.948   1.00   20.772   B   ATOM   2235   H   GLY   186   15.109   72.886   32.688   1.00   0.00   B   ATOM   2235   C   GLY   186   13.134   71.359   33.073   1.00   16.88   B   ATOM   2237   C   GLY   186   13.134   71.359   33.073   1.00   16.88   B   ATOM   2238   O   GLY   186   13.134   71.359   33.073   1.00   16.88   B   ATOM   2239   N   ILE   187   12.020   70.721   33.346   1.00   10.74   B   ATOM   2240   H   ILE   187   12.020   70.721   33.346   1.00   10.53   B   ATOM   2241   CA   ILE   187   11.152   71.172   33.346   1.00   0.00   B   ATOM   2242   CB   ILE   187   11.766   69.193   35.366   1.00   9.81   B   ATOM   2244   CG1   ILE   187   11.766   69.193   35.366   1.00   9.81   B   ATOM   2244   CG1   ILE   187   11.766   69.991   36.207   1.00   10.95   B   ATOM   2245   CD1   ILE   187   11.766   69.886   37.678   1.00   10.95   B   ATOM   2247   O   ILE   187   11.91   68.422   33.165   1.00   14.75   B   ATOM   2247   O   ILE   187   11.91   68.422   33.165   1.00   14.75   B   ATOM   2248   N   VAL   188   11.566   67.299   32.908   1.00   14.75   B   ATOM   2248   N   VAL   188   11.756   67.299   32.908   1.00   14.75   B   ATOM   2247   O   ILE   187   10.022   68.699   32.908   1.00   14.75   B   ATOM   2250   CA   VAL   188   11.756   67.299   32.696   1.00   20.73   B   ATOM   2250   CA   VAL   188   11.756   67.299   32.696   1.00   20.73   B   ATOM   2251   CB   VAL   188   11.363   64.610   30.107   1.00   17.83   B   ATOM   2252   CG1   VAL   188   11.363   64.610   30.620   1.00   17.83   B   ATOM   2255   CB   CML   188   11.363   64.610   30.107   1.00   17.83   B   ATOM   2255   CB   GLN   189   9.992   64.704   32.661   1.00   0.00   B   ATOM   2256   CG   GLN   189   9.993   63.076   33.742   1.00   2.92   B   ATOM   2255   CB   GLN   189   9.993   63.076   33.742   1.00   2.00   0.00   B   ATOM   2265   CB   GLN   189   9.993   63.076   33.742				CG1	VAL	185	15.608	73.149	35.795	1.00 14.91	В
35		MOTA	2231	CG2	VAL	185	17.641	74.610	35.686	1.00 13.27	В
ATOM   2234   N   GLY   186		MOTA	2232	C	VAL	185	14.411	74.506	33.614	1.00 16.98	В
ATOM 2235 H GLY 186 15.109 72.886 32.688 1.00 0.00 B ATOM 2236 CA GLY 186 13.016 72.794 32.585 1.00 14.37 B ATOM 2238 O GLY 186 13.134 71.359 33.073 1.00 16.88 B ATOM 2239 N ILE 187 12.020 70.721 33.409 1.00 12.53 B ATOM 2240 H ILE 187 11.152 71.172 33.346 1.00 0.00 B ATOM 2241 CA ILE 187 11.152 71.172 33.346 1.00 0.00 B ATOM 2241 CA ILE 187 11.152 71.172 33.346 1.00 10.78 B ATOM 2242 CB ILE 187 11.766 69.193 35.366 1.00 14.75 B ATOM 2244 CGI ILE 187 11.766 69.193 35.366 1.00 10.78 B ATOM 2244 CGI ILE 187 11.766 69.193 35.366 1.00 10.78 B ATOM 2245 CDI ILE 187 12.818 69.901 36.207 1.00 10.78 B ATOM 2245 CDI ILE 187 12.517 69.886 37.678 1.00 7.68 B ATOM 2245 CDI ILE 187 12.517 69.886 37.678 1.00 7.68 B ATOM 2245 CDI ILE 187 11.91 68.422 33.105 1.00 12.90 B ATOM 2247 O ILE 187 10.022 68.699 32.908 1.00 14.75 B ATOM 2248 N VAL 188 11.756 67.299 32.908 1.00 14.75 B ATOM 2248 N VAL 188 11.756 67.299 32.906 1.00 12.90 B ATOM 2251 CB VAL 188 11.748 65.977 30.620 1.00 18.34 B ATOM 2251 CB VAL 188 11.748 65.977 30.620 1.00 18.34 B ATOM 2251 CB VAL 188 11.363 64.610 30.107 1.00 17.83 B ATOM 2253 CG2 VAL 188 11.363 64.610 30.107 1.00 17.83 B ATOM 2253 CG2 VAL 188 11.363 64.610 30.107 1.00 17.83 B ATOM 2255 CD VAL 188 11.363 64.610 30.107 1.00 17.83 B ATOM 2255 CD VAL 188 11.363 64.610 30.107 1.00 17.83 B ATOM 2255 CD CA VAL 188 11.363 64.610 30.107 1.00 17.83 B ATOM 2255 CD CA VAL 188 11.363 64.610 30.107 1.00 17.83 B ATOM 2255 CD CA VAL 188 11.363 64.610 30.107 1.00 17.85 B ATOM 2255 CD GLN 189 9.929 64.704 32.661 1.00 0.00 B ATOM 2255 CD GLN 189 9.939 63.076 34.798 1.00 12.92 B ATOM 2256 N GLN 189 9.939 63.076 33.742 1.00 20.85 B ATOM 2256 CD GLN 189 9.939 63.076 34.798 1.00 17.85 B ATOM 2256 CD GLN 189 9.939 63.076 34.798 1.00 17.85 B ATOM 2266 CD GLN 189 9.939 63.076 33.7491 1.00 17.85 B ATOM 2267 CD GLN 189 9.939 63.076 33.7491 1.00 17.85 B ATOM 2268 N TYR 190 9.958 60.799 32.897 1.00 17.53 B ATOM 2268 N TYR 190 9.958 60.799 32.897 1.00 17.53 B ATOM 2267 CD GLN 189 9.9444 62.015 32.769 1.00 13.48 B ATOM 2269 H TYR 19	35	MOTA	2233	0	VAL	185	13.458				
ATOM 2236 CA GLY 186 13.016 72.794 32.585 1.00 14.37 B ATOM 2237 C GLY 186 13.134 71.359 33.073 1.00 16.88 B ATOM 2238 O GLY 186 14.252 70.825 33.165 1.00 10.74 B ATOM 2239 N ILE 187 12.020 70.721 33.409 1.00 12.53 B ATOM 2240 H ILE 187 12.104 69.344 33.346 1.00 0.00 B ATOM 2241 CA ILE 187 12.104 69.344 33.346 1.00 0.00 B ATOM 2241 CB ILE 187 12.104 69.344 33.369 1.00 14.75 B ATOM 2244 CGB ILE 187 11.766 69.193 35.366 1.00 9.81 B ATOM 2244 CGB ILE 187 11.766 69.193 35.366 1.00 10.78 B ATOM 2244 CGB ILE 187 12.818 69.901 36.207 1.00 10.78 B ATOM 2244 CGB ILE 187 12.818 69.901 36.207 1.00 10.78 B ATOM 2244 CGB ILE 187 12.517 69.886 37.678 1.00 10.95 B ATOM 2246 C ILE 187 11.91 68.422 33.105 1.00 12.90 B ATOM 2247 O ILE 187 10.022 68.699 32.908 1.00 14.75 B ATOM 2248 N VAL 188 11.756 67.299 32.908 1.00 14.75 B ATOM 2249 H VAL 188 11.756 67.299 32.908 1.00 14.75 B ATOM 2250 CA VAL 188 11.756 67.299 32.908 1.00 20.73 B ATOM 2251 CB VAL 188 11.040 66.267 31.970 1.00 18.34 B ATOM 2251 CB VAL 188 11.040 66.267 31.970 1.00 18.34 B ATOM 2252 CGI VAL 188 11.432 67.075 29.602 1.00 10.78 B ATOM 2255 CGI VAL 188 11.432 67.075 29.602 1.00 10.78 B ATOM 2255 CG VAL 188 11.432 67.075 29.602 1.00 10.78 B ATOM 2255 CG GLN 189 9.929 64.338 33.014 1.00 19.46 B ATOM 2255 CG GLN 189 9.929 64.338 33.014 1.00 19.46 B ATOM 2255 CG GLN 189 9.929 64.338 33.014 1.00 19.46 B ATOM 2255 CG GLN 189 9.938 63.076 33.742 1.00 20.85 B ATOM 2256 CG GLN 189 9.938 63.076 33.742 1.00 20.85 B ATOM 2261 CD GLN 189 9.939 63.076 34.980 1.00 16.55 B ATOM 2266 CG GLN 189 9.939 63.076 34.980 1.00 16.55 B ATOM 2266 CG GLN 189 9.939 63.076 33.742 1.00 20.55 B ATOM 2266 CG GLN 189 9.938 63.076 33.742 1.00 20.55 B ATOM 2266 CG GLN 189 9.938 63.076 33.742 1.00 20.55 B ATOM 2266 CG GLN 189 9.939 63.076 33.742 1.00 20.55 B ATOM 2266 CG GLN 189 9.939 63.076 33.742 1.00 20.55 B ATOM 2266 CG GLN 189 9.939 63.076 33.742 1.00 20.55 B ATOM 2266 CG GLN 189 9.939 63.076 33.593 1.00 10.00 B ATOM 2266 CG GLN 189 9.939 63.076 33.593 1.00 10.00 B ATOM 2267 O GLN 189 9.936 60.63		MOTA	2234	N	GLY						
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ATOM											
ATOM 2249 N ILE 187 12.020 70.721 33.409 1.00 12.53 B ATOM 2240 H ILE 187 11.152 71.172 33.346 1.00 0.00 B ATOM 2241 CA ILE 187 11.152 71.172 33.346 1.00 0.00 B ATOM 2241 CA ILE 187 12.104 69.344 33.869 1.00 14.75 B ATOM 2242 CB ILE 187 11.766 69.193 35.366 1.00 9.81 B ATOM 2243 CG2 ILE 187 11.733 67.712 35.742 1.00 10.78 B ATOM 2244 CG1 ILE 187 11.733 67.712 35.742 1.00 10.78 B ATOM 2244 CG1 ILE 187 12.818 69.901 36.207 1.00 10.95 B ATOM 2245 CD1 ILE 187 12.818 69.901 36.207 1.00 10.95 B ATOM 2246 C ILE 187 11.191 68.422 33.105 1.00 7.68 B ATOM 2247 O ILE 187 10.022 68.699 32.908 1.00 14.75 B ATOM 2248 N VAL 188 11.756 67.299 32.696 1.00 20.73 B ATOM 2249 H VAL 188 11.756 67.299 32.696 1.00 20.73 B ATOM 2250 CA VAL 188 11.040 66.267 31.970 1.00 18.34 B ATOM 2251 CB VAL 188 11.748 65.977 30.620 1.00 23.42 B ATOM 2251 CB VAL 188 11.748 65.977 30.620 1.00 23.42 B ATOM 2252 CG1 VAL 188 11.363 64.610 30.107 1.00 17.83 B ATOM 2254 C VAL 188 11.363 64.610 30.107 1.00 17.83 B ATOM 2255 O VAL 188 11.363 64.610 30.107 1.00 17.83 B ATOM 2255 CG VAL 188 11.363 64.610 30.107 1.00 17.83 B ATOM 2255 CG VAL 188 11.363 64.610 30.107 1.00 17.83 B ATOM 2255 CG VAL 188 11.363 64.610 30.107 1.00 17.83 B ATOM 2255 CG VAL 188 11.363 64.610 30.107 1.00 17.83 B ATOM 2255 CG GI VAL 188 11.363 64.610 30.107 1.00 17.83 B ATOM 2255 CG GI VAL 188 11.363 64.610 30.107 1.00 17.83 B ATOM 2255 CG GI VAL 188 11.007 64.992 32.831 1.00 22.16 B ATOM 2255 CG GI VAL 188 11.007 64.992 32.831 1.00 22.16 B ATOM 2256 N GLN 189 9.992 64.704 32.661 1.00 10.00 B ATOM 2256 CG GIN 189 9.993 63.076 34.980 1.00 10.655 B ATOM 2256 CG GIN 189 9.993 63.076 34.980 1.00 10.655 B ATOM 2256 CG GIN 189 9.993 63.076 34.980 1.00 10.655 B ATOM 2266 CG GIN 189 9.993 63.076 34.980 1.00 10.655 B ATOM 2266 CG GIN 189 8.294 60.553 37.608 1.00 17.85 B ATOM 2266 CG IN 189 9.993 63.076 34.980 1.00 10.555 B ATOM 2266 CG IN 189 9.993 63.076 34.980 1.00 10.555 B ATOM 2266 CG IN 189 9.993 60.0631 33.593 1.00 0.00 B ATOM 2266 F GLN 189 9.993 60.0631 33.593 1.00 0.00 B ATOM 2266 F GLN	40										
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ATOM         2247         O         ILE         187         10.022         68.699         32.908         1.00         14.75         B           ATOM         2248         N         VAL         188         11.756         67.299         32.696         1.00         20.73         B           ATOM         2249         H         VAL         188         12.703         67.157         32.892         1.00         0.00         B           ATOM         2251         CB         VAL         188         11.040         66.267         31.970         1.00         18.34         B           ATOM         2251         CB         VAL         188         11.748         65.977         30.620         1.00         17.83         B           55         ATOM         2252         CG1         VAL         188         11.363         64.610         30.107         1.00         17.83         B           55         ATOM         2253         CG2         VAL         188         11.077         64.992         32.831         1.00         12.92         B           ATOM         2255         O         VAL         188         12.126         64.630         33.37											
50         ATOM         2248         N         VAL         188         11.756         67.299         32.696         1.00         20.73         B           ATOM         2249         H         VAL         188         12.703         67.157         32.892         1.00         0.00         B           ATOM         2250         CA         VAL         188         11.040         66.267         31.970         1.00         18.34         B           ATOM         2251         CB         VAL         188         11.748         65.977         30.620         1.00         17.83         B           ATOM         2252         CG1         VAL         188         11.363         64.610         30.107         1.00         17.83         B           ATOM         2253         CG2         VAL         188         11.432         67.075         29.602         1.00         16.65         B           ATOM         2255         C         VAL         188         11.077         64.992         32.831         1.00         22.16         B           ATOM         2255         O         VAL         188         12.126         64.630         33.373         1											В
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	ATOM	2272	CG	TYR	190	11.882	58.859	31.318	1.00 24.13	В
	ATOM	2273	CD1	TYR	190	12.035	57.474	31.253	1.00 29.37	В
	ATOM	2274	CE1	TYR	190	13.194	56.859	31.702	1.00 26.64	B
	ATOM	2275		TYR	190	12.937	59.617	31.835	1.00 22.88	В
5	MOTA	2276		TYR	190	14.105	59.006	32.283	1.00 22.43	В
J	ATOM	2277	CZ	TYR	190	14.220	57.632	32.221	1.00 24.14	В
		2278	OH	TYR	190	15.330	57.013	32.741	1.00 25.80	В
	MOTA				190	15.251	56.064	32.618	1.00 0.00	В
	ATOM	2279	HH	TYR		9.346	58.474	32.860	1.00 17.06	В
4.0	MOTA	2280	C	TYR	190				1.00 19.81	В
10	MOTA	2281	0	TYR	190	9.753	58.408	34.027		В
	MOTA	2282	N	GLY	191	8.666	57.502	32.273	1.00 18.92	
	ATOM	2283	H	GLY	191	8.353	57.624	31.354	1.00 0.00	В
	MOTA	2284	$^{\rm CA}$	GLY	191	8.373	56.255	32.963	1.00 16.20	В
	ATOM	2285	С	GLY	191	7.278	55.625	32.137	1.00 17.90	В
15	ATOM	2286	0	GLY	191	6.100	55.732	32.480	1.00 34.36	В
10	ATOM	2287	N	GLU	192	7.672	54.993	31.041	1.00 16.02	В
	MOTA	2288	H	GLU	192	8.631	54.939	30.847	1.00 0.00	В
	MOTA	2289	CA	GLU	192	6.728	54.371	30.100	1.00 24.28	В
		2290	CB	GLU	192	5.433	53.920	30.798	1.00 31.95	В
20	ATOM			GLU	192	5.253	52.419	30.945	1.00 36.40	В
20	MOTA	2291	CG		192	4.309	52.063	32.084	1.00 46.73	В
	ATOM	2292	CD CT1	GLU			50.864	32.253	1.00 46.15	В
	MOTA	2293		GLU	192	3.996		32.233	1.00 50.61	В
	MOTA	2294	OE2	GLU	192	3.878	52.985	-	1.00 19.84	В
	MOTA	2295	С	GLU	192	6.397	55.450	29.077		В
25	MOTA	2296	0	$\operatorname{GLU}$	192	6.518	55.239	27.870	1.00 16.66	
	ATOM	2297	N	ASN	193	5.990	56.614	29.580	1.00 13.96	В
	ATOM	2298	H	ASN	193	5.913	56.713	30.550	1.00 0.00	В
	MOTA	2299	CA	ASN	193	5.659	57.750	28.722	1.00 18.10	В
	ATOM	2300	CB	ASN	193	4.150	58.065	28.785	1.00 17.15	В
30	ATOM	2301	CG	ASN	193	3.290	56.962	28.183	1.00 17.46	В
	MOTA	2302	OD1	ASN	193	3.165	56.857	26.965	1.00 24.21	В
	ATOM	2303	ND2	ASN	193	2.690	56.138	29.040	1.00 9.82	В
	ATOM	2304	HD21	ASN	193	2.815	56.262	30.004	1.00 0.00	В
	ATOM	2305	HD22	ASN	193	2.135	55.426	28.665	1.00 0.00	В
35	ATOM	2306	C	ASN	193	6.468	58.961	29.202	1.00 16.97	В
	ATOM	2307	0	ASN	193	7.080	58.918	30.280	1.00 19.37	В
	ATOM	2308	N	VAL	194	6.470	60.025	28.404	1.00 13.36	В
	ATOM	2309	H	VAL	194	5.964	59.992	27.567	1.00 0.00	В
	ATOM	2310	CA	VAL	194	7.204	61.250	28.734	1.00 18.46	В
40	ATOM	2311	CB	VAL	194	8.117	61.699	27.555	1.00 17.45	В
40	ATOM	2312		VAL	194	9.043	62.818	28.003	1.00 16.70	В
	ATOM	2313		VAL	194	8.901	60.526	27.022	1.00 11.05	В
	ATOM	2314	C	VAL	194	6.284	62.417	29.047	1.00 18.32	В
	MOTA	2315	Ö	VAL	194	5.377	62.710	28.273	1.00 17.95	В
45	MOTA	2316	N	THR	195	6.543	63.095	30.164	1.00 18.97	В
43		2317	H	THR	195	7.285	62.797	30.728	1.00 0.00	В
	MOTA	2317	CA	THR	195	5.768	64.265	30.582	1.00 20.52	В
	MOTA		CB	THR	195	5.012	63.982	31.906	1.00 18.21	В
	MOTA	2319				5.765	64.482	33.014	1.00 30.10	В
50	MOTA	2320	OG1		195		64.302	33.830	1.00 0.00	В
50	ATOM	2321		THR	195	5.291	62.510	32.091	1.00 23.60	В
	ATOM	2322	CG2		195	4.828	65.486	30.791	1.00 24.72	В
	ATOM	2323	C	THR	195	6.673		31.302	1.00 25.20	В
	ATOM	2324	0	THR	195	7.792	65.355		1.00 24.33	В
	MOTA	2325	N	$\mathtt{HIS}$	196	6.216	66.669	30.371		В
55	MOTA	2326	H	HIS	196	5.347	66.719	29.922	1.00 0.00	
	ATOM	2327	CA	HIS	196	6.997	67.890	30.576	1.00 20.06	В
	MOTA	2328	CB	HIS	196	6.787	68.891	29.438	1.00 20.11	В
	ATOM	2329	CG	HIS	196	7.414	68.468	28.144	1.00 31.04	В
	MOTA	2330		HIS	196	6.916	67.757	27.103	1.00 32.61	В
60	MOTA	2331		HIS	196	8.723	68.754	27.823	1.00 32.93	В
• •	ATOM	2332		HIS	196	9.343	69.258	28.384	1.00 0.00	В
	MOTA	2333		HIS	196	9.008	68.235	26.640	1.00 30.15	В
	ATOM	2334		HIS	196	7.929	67.625	26.183	1.00 29.88	В
	ATOM	2335		HIS	196	7.865	67.157	25.331	1.00 0.00	В
65	ATOM	2336		HIS	196	6.449	68.473	31.864	1.00 23.53	В
05	ATOM	2337		HIS	196	5.330	68.968	31.872	1.00 24.48	В
		2338		GLU	197	7.214	68.392	32.959	1.00 21.43	В
	ATOM	2339		GLU	197	8.101	67.980	32.898	1.00 0.00	В
	MOTA			GLU	197	6.745	68.908	34.244	1.00 21.98	В
70	ATOM	2340		GLU	197	7.635	68.416	35.385	1.00 22.07	В
70	ATOM	2341		GLU	197	7.553	66.900	35.626	1.00 22.26	В
	ATOM	2342			197	6.265	66.461	36.330	1.00 19.16	В
	MOTA	2343		GLU		5.436	67.324	36.655	1.00 21.45	В
	MOTA	2344	· OET	GLU	197	5.450	07.324	20.033	T.00 DI.43	

	ATOM	2345	OE2	GLU	197	6.080	65.252	36.559	1.00 25.81	В
	MOTA	2346	С	GLU	197	6.697	70.432	34.179	1.00 21.01	В
	ATOM ATOM	2347 2348	O N	GLU PHE	197 198	5.771 7.715	71.057 71.028	34.704 33.568	1.00 20.20 1.00 20.63	B B
5	ATOM	2349	H	PHE	198	8.475	70.486	33.270	1.00 0.00	В
	MOTA	2350	CA	PHE	198	7.733	72.465	33.329	1.00 16.85	В
	ATOM	2351 2352	CB CG	PHE PHE	198 198	7.846 9.077	73.321 73.099	34.618 35.447	1.00 19.79 1.00 18.93	B B
	MOTA MOTA	2353	CD1		198	10.282	73.736	35.134	1.00 15.68	В
10	MOTA	2354	CD2		198	9.003	72.358	36.619	1.00 17.58	В
	MOTA	2355	CE1		198 198	11.389 10.113	73.642 72.258	35.984 37.480	1.00 8.10 1.00 17.77	B B
	ATOM ATOM	2356 2357	CE2 CZ	PHE PHE	198	11.307	72.238	37.154	1.00 18.12	В
	MOTA	2358	C	PHE	198	8.773	72.827	32.285	1.00 23.38	В
15	MOTA	2359	0	PHE	198	9.848	72.210	32.191 31.457	1.00 19.68 1.00 22.68	B B
	ATOM ATOM	2360 2361	N H	ASN ASN	199 199	8.403 7.536	73.797 74.227	31.437	1.00 22.08	В
	ATOM	2362	CA	ASN	199	9.251	74.241	30.379	1.00 19.07	В
•	ATOM	2363	CB	ASN	199	8.402	74.980	29.342	1.00 18.17 1.00 16.13	B B
20	ATOM ATOM	2364 2365	CG OD1	ASN	199 199	7.545 7.520	74.033 72.824	28.511 28.741	1.00 16.13	В
	ATOM	2366	ND2		199	6.849	74.579	27.532	1.00 18.89	В
	MOTA	2367	HD21		199	6.902	75.547	27.376	1.00 0.00	В
25	ATOM		HD22	ASN ASN	199 199	6.292 10.434	73.989 75.094	26.986 30.832	1.00 0.00 1.00 15.04	B B
25	ATOM ATOM	2369 2370	С О	ASN	199	10.465	75.613	31.944	1.00 15.97	В
	ATOM	2371	N	LEU	200	11.414	75.189	29.935	1.00 20.27	В
	ATOM	2372	H	LEU	200 200	11.297 12.655	74.727 75.939	29.080 30.140	1.00 0.00 1.00 20.09	B B
30	ATOM ATOM	2373 2374	CA CB	LEU LEU	200	13.504	75.847	28.859	1.00 20.33	В
50	ATOM	2375	CG	LEU	200	15.000	75.481	28.771	1.00 19.69	В
	ATOM	2376		LEU	200	15.510 15.189	74.719 74.680	29.975 27.506	1.00 14.91 1.00 11.40	B B
	ATOM ATOM	2377 2378	CD2	LEU LEU	200 200	12.387	77.404	30.468	1.00 18.48	В
35	ATOM	2379	Ö	LEU	200	13.155	78.034	31.193	1.00 20.99	В
	ATOM	2380	N	ASN	201	11.295	77.949 77.403	29.940 29.382	1.00 13.45 1.00 0.00	B B
	MOTA MOTA	2381 2382	H CA	ASN ASN	201 201	10.701 10.978	79.350	30.190	1.00 22.91	В
	ATOM	2383	CB	ASN	201	10.645	80.061	28.877	1.00 23.93	В
40	ATOM	2384	CG	ASN	201	9.360	79.545 79.911	28.229 27.103	1.00 25.62 1.00 32.16	B B
	ATOM ATOM	2385 2386		ASN ASN	201 201	9.048 8.624	78.700	28.932	1.00 32.10	В
	ATOM		HD21		201	8.908	78.429	29.828	1.00 0.00	В
15	ATOM		HD22		201	7.801 9.826	78.368 79.549	28.519 31.162	1.00 0.00 1.00 24.74	B B
45	ATOM ATOM	2389 2390	С О	ASN ASN	201 201	9.828	80.664	31.329	1.00 21.74	В
	ATOM	2391	N	LYS	202	9.378	78.468	31.789	1.00 27.24	В
	ATOM	2392	H	LYS	202	9.806 8.261	77.604 78.527	31.615 32.735	1.00 0.00 1.00 28.50	B B
50	ATOM ATOM	2393 2394	CA CB	LYS LYS	202 202	7.936	77.122	33.249	1.00 35.35	В
50	ATOM	2395	CG	LYS	202	6.537	77.001	33.861	1.00 44.45	В
	MOTA	2396	CD	LYS	202	5.511	76.529	32.828	1.00 51.43 1.00 52.91	В В
	ATOM ATOM	2397 2398	CE NZ	LYS LYS	202 202	5.819 5.156	75.112 74.748	32.334 31.049	1.00 49.04	В
55	ATOM	2399		LYS	202	5.462	75.400	30.301	1.00 0.00	В
	ATOM	2400		LYS	202	4.124	74.807	31.163	1.00 0.00 1.00 0.00	В
	ATOM ATOM	2401 2402	HZ3 C	LYS LYS	202 202	5.419 8.450	73.774 79.451	30.788 33.934	1.00 0.00 1.00 25.89	B B
	ATOM	2402	0	LYS	202	7.550	80.227	34.260	1.00 25.05	В
60	ATOM	2404	N	TYR	203	9.617	79.348	34.577	1.00 22.72	В
	ATOM	2405	H	TYR	203	10.276 9.978	78.722 80.123	34.225 35.770	1.00 0.00 1.00 26.57	B B
	ATOM ATOM	2406 2407	CA CB	TYR TYR	203 203	10.246	79.166	36.937	1.00 20.51	В
	MOTA	2408	CG	TYR	203	9.065	78.303	37.215	1.00 23.59	В
65	MOTA	2409		TYR	203	9.075	76.941	36.901	1.00 24.81 1.00 23.81	В
	ATOM ATOM	2410 2411	CE1 CD2		203 203	7.927 7.886	76.163 78.870	37.057 37.706	1.00 23.81	В В
	ATOM	2411	CE2		203	6.741	78.113	37.871	1.00 28.83	В
	ATOM	2413	CZ	TYR	203	6.762	76.763	37.542	1.00 32.83	В
70	ATOM	2414	OH	TYR	203	5.598 5.758	76.043 75.133	37.683 37.423	1.00 29.24 1.00 0.00	В В
	ATOM ATOM	2415 2416	HH C	TYR TYR	203 203	11.201	81.013	35.569	1.00 27.09	В
	MOTA	2417		TYR	203	12.229	80.563	35.056	1.00 24.90	В

	ATOM	2418	N	SER	204	11.089	82.268	35.995	1.00 29.38	В
	ATOM	2419	H	SER	204	10.256	82.561	36.419	1.00 0.00	В
	ATOM	2420	CA	SER	204	12.189	83.216	35.845	1.00 29.68	В
	MOTA	2421	CB	SER	204	11.701	84.509	35.158	1.00 29.69	В
5		2421	OG	SER	204	10.458	84.974	35.668	1.00 34.41	В
3	MOTA				204	9.786	84.301	35.536	1.00 0.00	В
	ATOM	2423	HG	SER		12.917	83.547	37.150	1.00 30.79	В
	ATOM	2424	C	SER	204		84.642	37.314	1.00 30.73	В
	MOTA	2425	0	SER	204	13.453		38.074	1.00 28.19	В
	ATOM	2426	N	SER	205	12.934	82.587	37.903	1.00 28.19	В
10	MOTA	2427	H	SER	205	12.458	81.749		1.00 22.80	В
	MOTA	2428	CA	SER	205	13.642	82.755	39.334		В
	ATOM	2429	CB	SER	205	12.895	83.709	40.263	1.00 23.08	
	MOTA	2430	OG	SER	205	11.998	83.004	41.097	1.00 23.87	В
	MOTA	2431	$^{\mathrm{HG}}$	SER	205	11.543	83.623	41.672	1.00 0.00	В
15	MOTA	2432	C	SER	205	13.851	81.395	40.003	1.00 25.18	В
	MOTA	2433	0	SER	205	13.079	80.451	39.794	1.00 20.34	В
	MOTA	2434	N	THR	206	14.919	81.307	40.788	1.00 23.66	В
	MOTA	2435	H	THR	206	15. <b>4</b> 86	82.100	40.902	1.00 0.00	В
	MOTA	2436	CA	THR	206	15.289	80.086	41.487	1.00 27.98	В
20	MOTA	2437	CB	THR	206	16.678	80.229	42.129	1.00 26.89	В
20	ATOM	2438		THR	206	17.514	81.019	41.272	1.00 29.58	В
	ATOM	2439		THR	206	17.597	80.587	40.418	1.00 0.00	В
	ATOM	2440		THR	206	17.319	78.875	42.330	1.00 22.76	В
	ATOM	2441	C	THR	206	14.295	79.661	42.556	1.00 29.88	B
25		2442	0	THR	206	14.057	78.457	42.730	1.00 24.79	В
23	ATOM	2442		GLU	207	13.713	80.626	43.274	1.00 29.47	В
	ATOM		N		207	13.932	81.567	43.109	1.00 0.00	В
	ATOM	2444	H	GLU		12.746	80.266	44.308	1.00 32.79	В
	MOTA	2445	CA	GLU	207	12.740	81.492	45.089	1.00 32.73	В
20	MOTA	2446	CB	GLU	207		82.875	44.665	1.00 45.27	B
30	MOTA	2447	CG	GLU	207	12.696			1.00 43.27	В
	MOTA	2448	CD	GLU	207	11.738	84.002	45.104		В
	ATOM	2449		GLU	207	11.106	84.632	44.220	1.00 49.46	В
	MOTA	2450		GLU	207	11.618	84.260	46.330	1.00 48.25	
	ATOM	2451	С	GLU	207	11.582	79.567	43.623	1.00 30.36	В
35	MOTA	2452	0	$\operatorname{GLU}$	207	11.141	78.499	44.052	1.00 29.14	В
	MOTA	2453	N	GLU	208	11.108	80.172	42.538	1.00 30.06	В
	ATOM	2454	H	$\operatorname{GLU}$	208	11.527	81.005	42.237	1.00 0.00	В
	ATOM	2455	CA	$\operatorname{GLU}$	208	9.980	79.635	41.781	1.00 24.26	В
	MOTA	2456	CB	$\operatorname{GLU}$	208	9.588	80.606	40.680	1.00 25.42	В
40	MOTA	2457	CG	GLU	208	8.833	81.818	41.198	1.00 32.20	В
	MOTA	2458	CD	GLU	208	8.830	82.953	40.203	1.00 37.03	В
	MOTA	2459	OE1	GLU	208	7.763	83.243	39.623	1.00 39.29	В
	MOTA	2460	OE2	GLU	208	9.900	83.551	40.000	1.00 39.74	В
	ATOM	2461	С	GLU	208	10.223	78.265	41.174	1.00 20.07	В
45	ATOM	2462	0	GLU	208	9.308	77.465	41.049	1.00 24.58	В
	ATOM	2463	N	VAL	209	11.459	78.000	40.783	1.00 17.97	В
	ATOM	2464	H	VAL	209	12.154	78.681	40.891	1.00 0.00	В
	ATOM	2465	CA	VAL	209	11.798	76.715	40.198	1.00 15.42	В
	ATOM	2466	CB	VAL	209	13.158	76.797	39.466	1.00 18.29	В
50	ATOM	2467		VAL	209	13.810	75.418	39.380	1.00 13.02	В
50	ATOM	2468		VAL	209	12.946	77.399	38.087	1.00 13.44	В
	ATOM	2469	C	VAL	209	11.860	75.669	41.308	1.00 16.08	В
	ATOM	2470	Ö	VAL	209	11.460	74.521	41.110	1.00 17.96	В
		2471	N	LEU	210	12.345	76.074	42.480	1.00 23.26	В
55	MOTA				210	12.643	77.004	42.575	1.00 0.00	В
55	MOTA	2472	H	LEU		12.445	75.166	43.626	1.00 24.65	В
	MOTA	2473	CA	LEU	210	13.202	75.824	44.777	1.00 19.16	B
	ATOM	2474	CB	LEU	210		75.955	44.603	1.00 29.23	В
	ATOM	2475	CG	LEU	210	14.712		45.687	1.00 32.84	В
	MOTA	2476		LEU	210	15.270	76.886		1.00 32.84	В
60	MOTA	2477		LEU	210	15.354	74.576	44.682	1.00 27.07	В
	MOTA	2478	C	LEU	210	11.051	74.805	44.099		
	MOTA	2479	0	$_{ m LEU}$	210	10.790	73.690	44.555	1.00 24.27	В
	ATOM	2480	N	VAL	211	10.150	75.770	44.012	1.00 27.55	В
	MOTA	2481	H	VAL	211	10.408	76.654	43.678	1.00 0.00	В
65	MOTA	2482	CA	VAL	211	8.787	75.518	44.414	1.00 24.35	В
	ATOM	2483	CB	VAL	211	7.966	76.832	44.404	1.00 23.80	В
	ATOM	2484		VAL	211	6.474	76.535	44.344	1.00 22.78	В
	ATOM	2485		VAL	211	8.292	77.641	45.661	1.00 20.18	В
	ATOM	2486	C	VAL	211	8.176	74.472	43.472	1.00 24.70	В
70	ATOM	2487	Ö	VAL	211	7.566	73.504	43.934	1.00 24.21	В
, 0	ATOM	2488	N	ALA	212	8.364	74.643	42.163	1.00 24.07	В
	ATOM	2489	H	ALA	212	8.883	75.411	41.847	1.00 0.00	В
		2490	CA	ALA	212	7.806	73.695	41.183	1.00 23.91	В
	MOTA	24JU	CA	עיייני	414					

	ATOM	2491 CB AL		8.004	74.221	39.777	1.00 20.84	В
	ATOM	2492 C AL		8.416	72.299	41.279	1.00 23.54	В
	ATOM	2493 O AL		7.709	71.280	41.195	1.00 19.74 1.00 22.17	B B
~	MOTA	2494 N AL		9.736	72.270 73.119	41.433 41.495	1.00 22.17	B
5	ATOM	2495 H AL		10.220 $10.484$	71.032	41.516	1.00 20.06	В
	MOTA	2496 CA AL. 2497 CB AL.		11.966	71.332	41.523	1.00 23.28	В
	ATOM	2497 CB AL. 2498 C AL.		10.096	70.259	42.763	1.00 24.35	B
	ATOM ATOM	2499 O AL		10.032	69.034	42.748	1.00 24.95	В
10	ATOM	2500 N AS		9.819	70.969	43.844	1.00 24.25	В
10	ATOM	2500 N AS		9.875	71.949	43.812	1.00 0.00	В
	ATOM	2502 CA AS		9.434	70.304	45.086	1.00 24.82	В
	ATOM	2503 CB AS		9.604	71.247	46.273	1.00 26.46	В
	ATOM	2504 CG AS		10.981	71.151	46.882	1.00 28.78	В
15	MOTA	2505 OD1 AS		11.870	71.958	46.578	1.00 23.63	В
	ATOM	2506 ND2 AS	v 214	11.179	70.153	47.739	1.00 25.69	В
	MOTA	2507 HD21 AS	v 214	10.444	69.533	47.941	1.00 0.00	В
	MOTA	2508 HD22 AS		12.063	70.070	48.145	1.00 0.00	В
	MOTA	2509 C AS		8.013	69.755	45.069	1.00 24.64	В
20	MOTA	2510 O AS		7.606	69.021	45.974	1.00 18.78	В
	ATOM	2511 N LY		7.256	70.103	44.039	1.00 23.65	B B
	MOTA	2512 H LY		7.617	70.696	43.345	1.00 0.00 1.00 26.33	B B
	ATOM	2513 CA LY		5.901	69.609 70.746	43.933 43.526	1.00 20.33	В
25	ATOM	2514 CB LY		4.961	71.337	44.708	1.00 22.32	В
25	MOTA	2515 CG LY		4.196 3.432	72.606	44.706	1.00 20.33	В
	MOTA	2516 CD LY		1.978	72.307	43.951	1.00 32.67	В
	MOTA MOTA	2517 CE LY 2518 NZ LY		1.649	72.846	42.601	1.00 35.42	В
	ATOM	2519 HZ1 LY		2.271	72.406	41.892	1.00 0.00	В
30	ATOM	2520 HZ2 LY		1.791	73.875	42.596	1.00 0.00	В
50	ATOM	2521 HZ3 LY		0.658	72.630	42.375	1.00 0.00	В
	MOTA	2522 C LY		5.760	68.434	42.960	1.00 22.45	В
	MOTA	2523 O LY		4.662	67.926	42.764	1.00 30.36	В
	MOTA	2524 N IL	E 216	6.864	67.976	42.375	1.00 16.84	В
35	MOTA	2525 H IL	E 216	7.734	68.373	42.593	1.00 0.00	В
	MOTA	2526 CA IL		6.781	66.884	41.415	1.00 12.02	В
	MOTA	2527 CB II	_	8.023	66.856	40.498	1.00 14.58	В
	MOTA	2528 CG2 II		8.050	65.566	39.671	1.00 19.30	B B
4.0	MOTA	2529 CG1 II		8.007	68.084	39.574 38.904	1.00 13.98 1.00 13.34	В
40	MOTA	2530 CD1 II		9.345	68.390 65.514	42.061	1.00 13.34	В
	ATOM	2531 C II		6.586 7.311	65.135	42.001	1.00 12.93	В
	MOTA	2532 O II 2533 N GI		5.581	64.785	41.580	1.00 17.89	В
	MOTA MOTA	2533 N GI 2534 H GI		5.022	65.150	40.868	1.00 0.00	В
45	ATOM	2535 CA GI		5.304	63.452	42.103	1.00 17.34	В
73	ATOM	2536 C GI		5.749	62.385	41.112	1.00 14.75	В
	ATOM	2537 O GI		5.675	62.588	39.898	1.00 15.21	В
	ATOM	2538 N AF		6.207	61.248	41.631	1.00 14.09	В
	ATOM	2539 H AF	G 218	6.226	61.146	42.604	1.00 0.00	В
50	ATOM	2540 CA AF	G 218	6.683	60.152	40.797	1.00 17.47	В
	MOTA	25 <b>4</b> 1 CB AF		7.195	59.023	41.707	1.00 21.57	В
	MOTA	2542 CG AF		6.442	57.725	41.637	1.00 25.79	В
	MOTA	2543 CD AF		7.384	56.563	41.388	1.00 22.17 1.00 16.26	B B
	MOTA	2544 NE A		7.509	55.752	42.588 42.782	1.00 10.20	В
55	MOTA	2545 HE AF		6.793	55.112 55.814	43.431	1.00 16.32	В
	ATOM	2546 CZ AF		8.531 9.521	56.644	43.210	1.00 28.95	В
	ATOM	2547 NH1 AF		9.511	57.229	42.399	1.00 0.00	В
	MOTA	2548 HH11 AI 2549 HH12 AI	G 218	10.287	56.689	43.849	1.00 0.00	В
60	MOTA MOTA	2550 NH2 A		8.546	55.054	44.512	1.00 33.70	В
00	ATOM	2551 HH21 A		7.789	54.425	44.693	1.00 0.00	В
	ATOM	2552 HH22 AI	G 218	9.316	55.104	45.146	1.00 0.00	В
	ATOM	2553 C AI		5.533	59.701	39.912	1.00 14.35	В
	ATOM	2554 O AI		4.524	59.251	40.405	1.00 19.15	В
65	ATOM	2555 N GI		5.670	59.815	38.597	1.00 17.48	В
	ATOM	2556 H GI		6.506	60.148	38.210	1.00 0.00	В
	ATOM		N 219	4.552	59.438	37.749	1.00 26.72	В
	MOTA	2558 CB G	N 219	4.664	60.107	36.363	1.00 23.72	В
	MOTA		N 219	5.223	59.280	35.221	1.00 25.69	В
70	MOTA	2560 CD G	JN 219	5.649	60.171	34.056	1.00 33.29	В
	MOTA	2561 OE1 G				34.257	1.00 26.70	В
	ATOM	2562 NE2 G				32.832 32.720	1.00 18.76 1.00 0.00	B B
	MOTA	2563 HE21 G	N 219	5.360	58.692	JZ.14U	1.00 0.00	מ

	MOTA	2564	HE22 (	GLN	219		5.906	60.191	32.081	1.00 0.00	В
	MOTA	2565		$\operatorname{GLN}$	219		4.344	57.935	37.650	1.00 26.26	В
	MOTA	2566		GLN	219		3.210	57.475	37.527	1.00 30.40 1.00 26.30	B B
_	MOTA	2567		GLY	220		5.419 6.305	57.166 57.568	37.745 37.863	1.00 20.30	В
5	MOTA	2568 2569		GLY GLY	220 220		5.270	55.728	37.672	1.00 30.10	В
	MOTA MOTA	2570		GLY	220		5.364	55.123	36.282	1.00 29.97	В
	MOTA	2571		GLY	220		5.002	55.740	35.277	1.00 33.59	В
	ATOM	2572		GLY	221		5.849	53.889	36.244	1.00 35.79	В
10	ATOM	2573		GLY	221		6.109	53.453	37.082	1.00 0.00	В
	ATOM	2574		GLY	221		6.004	53.171	34.998	1.00 39.72	В
	MOTA	2575	C	GLY	221		6.406	51.736	35.283	1.00 40.82	В
	MOTA	2576	0	$\operatorname{GLY}$	221		7.085	51.463	36.277	1.00 41.96	В
	MOTA	2577		LEU	222		5.974	50.822	34.422	1.00 37.83	В В
15	MOTA	2578		LEU	222		5.424	51.109	33.665 34.564	1.00 0.00 1.00 41.13	B
	ATOM	2579		LEU	222 222		6.288 5.102	49.402 48.543	34.103	1.00 42.69	В
	MOTA	2580 2581		LEU LEU	222		4.467	47.593	35.126	1.00 48.06	B
	ATOM ATOM	2582	CD1		222		4.063	48.361	36.380	1.00 47.26	В
20	ATOM	2583	CD2		222		3.259	46.917	34.509	1.00 44.76	В
20	MOTA	2584		LEU	222		7.506	49.093	33.707	1.00 39.93	В
	ATOM	2585		LEU	222		8.193	48.099	33.931	1.00 42.67	В
	MOTA	2586	N	GLN	223		7.755	49.954	32.723	1.00 35.86	В
	MOTA	2587		GLN	223		7.145	50.711	32.601	1.00 0.00	В
25	MOTA	2588		GLN	223		8.893	49.825	31.815	1.00 35.26 1.00 37.16	B B
	MOTA	2589		GLN	223		8.419	49.479	30.396 30.328	0.01 41.99	В
	MOTA	2590		GLN	223 223		6.995 6.839	48.952 47.821	29.332	0.01 44.07	В
	ATOM ATOM	2591 2592		GLN GLN	223		7.368	46.726	29.528	0.01 45.41	В
30	ATOM	2593		GLN	223		6.109	48.080	28.253	0.01 44.90	В
50	ATOM	2594		GLN	223		5.707	48.966	28.138	1.00 0.00	В
	ATOM	2595		GLN	223		5.997	47.364	27.601	1.00 0.00	В
	ATOM	2596		GLN	223		9.642	51.160	31.799	1.00 32.91	В
	ATOM	2597	0	GLN	223		9.032	52.218	31.641	1.00 24.75	В
35	MOTA	2598		THR	224		0.961	51.096	31.969	1.00 30.99	В
	MOTA	2599		THR	224		1.378	50.218	32.084 31.989	1.00 0.00 1.00 25.14	B B
	ATOM	2600		THR	224		1.814	52.283 52.047	32.891	1.00 23.14	В
	MOTA	2601	CB OG1	THR	$\frac{224}{224}$		2.548	51.636	34.177	1.00 22.14	В
40	ATOM ATOM	2602 2603		THR	224		2.042	50.826	34.091	1.00 0.00	В
40	ATOM	2604	CG2		224		3.850	53.315	33.025	1.00 16.21	В
	ATOM	2605	C	THR	224		2.295	52.644	30.590	1.00 24.48	В
	ATOM	2606	Ō	THR	224	1	3.197	52.010	30.042	1.00 22.45	В
	MOTA	2607	N	MET	225		1.695	53.688	30.027	1.00 23.62	В
45	MOTA	2608	H	MET	225		1.019	54.182	30.535	1.00 0.00	В
	MOTA	2609		MET	225		.2.015	54.118	28.673	1.00 21.06	B B
	MOTA	2610	CB	MET	225	ı	0.708	54.410 53.257	27.944 28.063	1.00 20.28	В
	MOTA	2611 2612	CG SD	MET MET	225 225	1	0.320	51.746	27.262	1.00 25.64	В
50	ATOM ATOM	2613	CE	MET	225		0.098	52.166	25.621	1.00 19.80	В
50	ATOM	2614	C	MET	225		2.943	55.327	28.629	1.00 20.97	В
	ATOM	2615	Õ	MET	225		2.562	56.408	28.185	1.00 23.42	В
	ATOM	2616	N	THR	226		4.177	55.119	29.062	1.00 22.97	В
	ATOM	2617	H	THR	226		4.433	54.221	29.359	1.00 0.00	В
55	ATOM	2618	CA	THR	226		.5.163	56.187	29.111	1.00 18.05	В
	MOTA	2619	CB	THR	226		6.487	55.667	29.700	1.00 20.16	В
	ATOM	2620	OG1		226		16.212	54.950	30.912	1.00 13.45	В
	ATOM	2621	HG1		226		15.789	55.535	31.542	1.00 0.00 1.00 15.25	B B
<b>60</b>	ATOM	2622		THR	226		L7.418	56.826	30.012 27.767	1.00 13.23	В
60	ATOM	2623	C	THR	226		L5.411 L5.468	56.836 58.059	27.787	1.00 17.23	В
	MOTA	2624	O	THR	226 227		L5.546	56.028	26.717	1.00 13.67	В
	ATOM	2625 2626	N H	ALA ALA	227		L5.502	55.057	26.849	1.00 0.00	В
	MOTA MOTA	2627	CA	ALA	227		15.768	56.558	25.381	1.00 14.13	В
65	ATOM	2628	CB	ALA	227		16.028	55.431	24.382	1.00 5.26	В
05	MOTA	2629	C	ALA	227		14.625	57.430	24.879	1.00 20.64	В
	ATOM	2630	Õ	ALA	227		14.862	58.332	24.067	1.00 30.73	В
	MOTA	2631	N	LEU	228		13.396	57.142	25.323	1.00 24.49	В
	ATOM	2632	H	LEU	228		L3.283	56.379	25.927	1.00 0.00	В
70	ATOM	2633	CA	LEU	228		L2.208	57.920	24.948	1.00 20.92	В
	MOTA	2634		LEU	228		10.918	57.301	25.507	1.00 28.56	В
	MOTA	2635		LEU	228		9.604	57.195	24.708	1.00 36.02	B B
	MOTA	2636	CD1	LEU	228		8.424	57.532	25.623	1.00 32.15	В

	ATOM	2637	CD2	LEU	228	9.615	58.114	23.504	1.00 38.46	В
	ATOM	2638	C	LEU	228	12.349	59.295	25.577	1.00 20.10	В
	MOTA	2639	0	LEU	228	12.252	60.307	24.894	1.00 21.88 1.00 17.67	B B
-	MOTA	2640	И	GLY	229	12.551	59.309 58.462	26.895 27.383	1.00 17.67	В
5	MOTA	2641 2642	H	GLY GLY	229 229	12.605 12.692	60.562	27.503	1.00 17.97	В
	ATOM ATOM	2643	CA C	GLY	229	13.757	61.507	27.070	1.00 16.62	В
	ATOM	2644	0	GLY	229	13.513	62.691	26.912	1.00 16.95	В
	ATOM	2645	N	THR	230	14.934	60.964	26.780	1.00 14.32	В
10	ATOM	2646	H	THR	230	15.056	60.004	26.924	1.00 0.00	В
	MOTA	2647	CA	THR	230	16.052	61.731	26.255	1.00 13.65	В
	ATOM	2648	CB	THR	230	17.311	60.832	26.166	1.00 13.38	В
	MOTA	2649	OG1		230	17.904	60.705	27.472	1.00 24.82	B B
1.7	ATOM	2650	HG1	THR	230	18.154	61.573 61.413	27.796 25.195	1.00 0.00 1.00 16.39	В
15	ATOM	2651	CG2	THR	230 230	18.331 15.722	62.276	24.865	1.00 16.56	В
	ATOM ATOM	2652 2653	С О	THR THR	230	15.923	63.452	24.580	1.00 14.40	B
	ATOM	2654	N	ASP	231	15.223	61.400	24.008	1.00 11.84	В
	MOTA	2655	H	ASP	231	15.086	60.475	24.300	1.00 0.00	В
20	MOTA	2656	CA	ASP	231	14.874	61.768	22.658	1.00 20.60	В
	MOTA	2657	CB	ASP	231	14.400	60.521	21.911	1.00 23.12	В
	MOTA	2658	CG	ASP	231	14.401	60.703	20.421	1.00 23.62	B B
	MOTA	2659	OD1		231	15.451	61.103	19.881 19.788	1.00 26.06 1.00 19.93	В
25	ATOM	2660	OD2		231 231	13.363 13.772	60.450 62.832	22.663	1.00 21.87	В
25	MOTA MOTA	2661 2662	C O	ASP ASP	231	13.800	63.799	21.898	1.00 20.06	В
	ATOM	2663	N	THR	232	12.804	62.637	23.544	1.00 22.80	В
	ATOM	2664	H	THR	232	12.854	61.855	24.132	1.00 0.00	В
	ATOM	2665	CA	THR	232	11.670	63.537	23.681	1.00 22.51	В
30	MOTA	2666	CB	THR	232	10.622	62.891	24.609	1.00 16.89	В
	MOTA	2667	OG1		232	10.277	61.607	24.075	1.00 21.61	В
	ATOM	2668	HG1	THR	232	11.061	61.055 63.733	24.031 24.706	1.00 0.00 1.00 20.59	B B
	MOTA	2669	CG2	THR THR	232 232	9.372 12.115	64.903	24.700	1.00 25.12	В
35	MOTA MOTA	2670 2671	С О	THR	232	11.601	65.952	23.782	1.00 25.24	В
22	MOTA	2672	N	ALA	233	13.091	64.882	25.098	1.00 21.55	В
	ATOM	2673	H	ALA	233	13.457	64.019	25.383	1.00 0.00	В
	MOTA	2674	CA	ALA	233	13.635	66.099	25.674	1.00 17.44	В
	MOTA	2675	CB	ALA	233	14.498	65.746	26.865	1.00 17.88	В
40	ATOM	2676	C	ALA	233	14.453	66.855	24.624 24.533	1.00 19.30 1.00 18.02	В В
	ATOM	2677	0	ALA	233 234	14.394 15.197	68.075 66.115	23.815	1.00 13.02	В
	ATOM ATOM	2678 2679	N H	ARG ARG	234	15.196	65.141	23.918	1.00 0.00	В
	ATOM	2680	CA	ARG	234	16.008	66.723	22.774	1.00 23.98	В
45	ATOM	2681	CB	ARG	234	16.857	65.647	22.087	1.00 25.23	В
	MOTA	2682	CG	ARG	234	17.603	66.121	20.851	1.00 28.43	В
	ATOM	2683	CD	ARG	234	18.028	64.952	19.994	1.00 25.37	В
	ATOM	2684	NE	ARG	234	17.098	64.763	18.887	1.00 35.93	В В
50	ATOM	2685	HE	ARG	234	16.794 $16.642$	65.558 63.584	18.403 18.494	1.00 0.00 1.00 33.70	В
50	ATOM	2686 2687	CZ NILI1	ARG ARG	234 234	17.036	62.484	19.120	1.00 42.49	В
	ATOM ATOM		HH11		234	17.678	62.545	19.883	1.00 0.00	В
	ATOM		HH12		234	16.693	61.592	18.824	1.00 0.00	В
	ATOM	2690		ARG	234	15.786	63.507	17.488	1.00 34.51	В
55	MOTA	2691	HH21	ARG	234	15.485	64.341	17.023	1.00 0.00	В
	MOTA		HH22		234	15.439	62.618	17.192	1.00 0.00	В
	MOTA	2693	C	ARG	234	15.071	67.341	21.747 $21.327$	1.00 23.74 1.00 19.58	B B
	ATOM	2694	0	ARG	234 235	15.212 14.099	68.500 66.535	21.327	1.00 19.38	В
60	MOTA	2695 2696	N H	LYS LYS	235	14.031	65.650	21.771	1.00 0.00	B
00	MOTA ATOM	2697	CA	LYS	235	13.136	66.915	20.349	1.00 23.75	В
	ATOM	2698	CB	LYS	235	12.365	65.674	19.907	1.00 27.18	В
	ATOM	2699	CG	LYS	235	12.541	65.347	18.434	1.00 39.17	В
	ATOM	2700	CD	LYS	235	12.592	63.848	18.206	1.00 40.05	В
65	MOTA	2701	CE	LYS	235	11.203	63.255	18.179	1.00 37.98	В
	ATOM	2702	NZ	LYS	235	11.172	62.081	17.280	1.00 36.28	В В
	ATOM	2703		LYS	235	11.846	61.365 62.374	17.624 16.319	1.00 0.00	В
	ATOM	2704		LYS	235 235	11.440 $10.215$	61.679	17.267	1.00 0.00	В
70	ATOM ATOM	2705 2706	HZ3	LYS LYS	235	12.159	67.992	20.776	1.00 14.66	В
70	ATOM	2700	0	LYS	235	11.854	68.867	20.003	1.00 15.35	В
	ATOM	2708	N	GLU	236	11.698	67.938	22.017	1.00 19.61	В
	MOTA	2709		GLU	236	12.029	67.243	22.621	1.00 0.00	В

	ATOM	2710	CA (	GLU	236	10.714	68.893	22.491	1.00 19.56	В
	ATOM	2711	CB (	GLU	236	9.467	68.131	22.980	1.00 17.41	В
	MOTA	2712	CG (	GLU	236	8.705	67.442	21.848	1.00 12.51	В
	MOTA	2713		GLU	236	7.734	66.365	22.326	1.00 20.23	В
5	MOTA	2714		GLU	236	7.147	66.493	23.416	1.00 16.25	B B
	ATOM	2715	OE2		236	7.553	65.382	21.594	1.00 32.75	В
	MOTA	2716		GLU	236	11.134	69.905	23.552 23.477	1.00 19.85 1.00 22.57	В
	ATOM	2717		GLU	236	$10.740 \\ 11.923$	71.074 69.477	24.530	1.00 13.82	В
10	ATOM	2718		ALA	237 237	12.243	68.552	24.528	1.00 0.00	В
10	ATOM ATOM	2719 2720		ALA ALA	237	12.320	70.380	25.609	1.00 15.91	В
	ATOM	2721		ALA	237	13.031	69.599	26.715	1.00 12.47	В
	ATOM	2722		ALA	237	13.183	71.568	25.185	1.00 18.22	В
	ATOM	2723		ALA	237	13.067	72.647	25.754	1.00 20.95	В
15	MOTA	2724		PHE	238	14.050	71.372	24.202	1.00 20.05	В
	MOTA	2725	H	PHE	238	14.094	70.495	23.767	1.00 0.00	В
	MOTA	2726	CA	PHE	238	14.938	72.443	23.757	1.00 25.75	В
	MOTA	2727		PHE	238	16.286	71.864	23.411	1.00 21.10	В
	MOTA	2728		PHE	238	17.058	71.430	24.607	1.00 20.59 1.00 10.70	B B
20	MOTA	2729	CD1		238	17.153 17.690	70.081 72.378	24.926 25.425	1.00 10.70	В
	ATOM	2730	CD2 CE1		238 238	17.865	69.668	26.043	1.00 6.53	В
	ATOM ATOM	2731 2732	CE2		238	18.407	71.981	26.548	1.00 9.67	В
	ATOM	2732		PHE	238	18.498	70.623	26.860	1.00 14.30	В
25	MOTA	2734		PHE	238	14.364	73.171	22.570	1.00 32.55	В
20	ATOM	2735		PHE	238	15.050	73.472	21.591	1.00 34.64	В
	ATOM	2736	N	THR	239	13.080	73.446	22.682	1.00 33.09	В
	ATOM	2737	H	THR	239	12.608	73.176	23.499	1.00 0.00	В
	ATOM	2738	CA	THR	239	12.344	74.125	21.651	1.00 37.89 1.00 34.14	B B
30	ATOM	2739	CB	THR	239	10.911 10.907	73.562 72.378	21.597 20.797	1.00 34.14	В
	MOTA	2740 2741	OG1 HG1		239 239	10.019	72.020	20.758	1.00 0.00	В
	MOTA MOTA	2741	CG2		239	9.953	74.558	21.010	1.00 42.52	В
	ATOM	2743	C	THR	239	12.329	75.606	21.986	1.00 38.96	В
35	ATOM	2744	0	THR	239	12.421	75.989	23.156	1.00 40.40	В
	ATOM	2745	N	GLU	240	12.229	76.438	20.962	1.00 36.75	В
	MOTA	2746	H	GLU	240	12.181	76.087	20.049	1.00 0.00 1.00 <b>42.</b> 75	B B
	MOTA	2747	CA	GLU	240	12.191 $12.344$	77.867 78.604	21.185 19.855	1.00 42.73	В
40	ATOM	2748 2749	CB CG	GLU GLU	240 240	11.038	78.872	19.148	1.00 62.98	В
40	ATOM ATOM	2750	CD	GLU	240	10.313	80.068	19.724	1.00 67.81	В
	MOTA	2751			240	10.925	81.156	19.774	1.00 70.98	В
	ATOM	2752	OE2		240	9.140	79.916	20.131	1.00 69.99	В
	ATOM	2753	С	GLU	240	10.843	78.178	21.843	1.00 40.19	В
45	ATOM	2754	0	GLU	240	10.751	79.041	22.707	1.00 33.66 1.00 33.98	B B
	ATOM	2755	N	ALA	241	9.804 9.936	77. <b>4</b> 58 76.796	21.423 20.714	1.00 33.98	В
	ATOM	2756 2757	H CA	ALA ALA	241 241	8.471	77.636	21.986	1.00 29.60	В
	ATOM ATOM	2758	CB	ALA	241	7.492	76.687	21.316	1.00 37.19	В
50	MOTA	2759	C	ALA	241	8.499	77.375	23.491	1.00 29.07	В
20	ATOM	2760	0	ALA	241	7.801	78.047	24.251	1.00 32.90	В
	MOTA	2761	N	ARG	242	9.312	76.406	23.916	1.00 25.07	В
	MOTA	2762	H	ARG	242	9.845	75.913	23.257	1.00 0.00	B
<i></i>	ATOM	2763	CA	ARG	242	9.429	76.057 74.551	25.332 25.495	1.00 21.30 1.00 21.86	B B
55	ATOM	2764	CB	ARG	242 242	9.644 8.486	73.680	24.980	1.00 18.40	В
	ATOM ATOM	2765 2766	CG CD	ARG ARG	242	8.520	72.317	25.663	1.00 23.54	В
	ATOM	2767	NE	ARG	242	7.674	71.334	25.001	1.00 27.29	В
	ATOM	2768	HE	ARG	242	7.958	70.990	24.131	1.00 0.00	В
60	ATOM	2769	CZ	ARG	242	6.536	70.870	25.509	1.00 21.77	В
	MOTA	2770		ARG	242	6.106	71.302	26.686	1.00 28.61	В
	ATOM		HH11		242	6.637	71.979	27.196	1.00 0.00	B B
	ATOM		HH12		242	5.249	70.952 69.967	27.064 24.851	1.00 0.00 1.00 21.18	В
65	ATOM	2773		ARG	242 242	5.842 6.171	69.625	23.969	1.00 0.00	В
65	ATOM ATOM		HH21 HH22		242	4.986	69.618	25.232	1.00 0.00	В
	ATOM	2776	C	ARG	242	10.538	76.806	26.071	1.00 17.43	В
	MOTA	2777	Õ	ARG	242	10.884	76.462	27.206	1.00 14.43	В
	ATOM	2778	И	GLY	243	11.127	77.800	25.419	1.00 15.32	В
70	MOTA	2779	H	$\operatorname{GLY}$	243	10.878	78.002	24.495	1.00 0.00	В
	MOTA	2780	CA	GLY	243	12.146	78.595	26.096	1.00 16.02	B B
	MOTA	2781	C	GLY	243	13.628	78.505 79.182	25.786 26.444	1.00 10.54	В
	MOTA	2782	0	$\operatorname{GLY}$	243	14.406	17.104	40.444	1.00 20.00	

5 10 15	ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2783 2784 2785 2786 2787 2788 2790 2791 2792 2793 2794 2795 2796 2797 2798 2799 2800 2800 2802	HH12 NH2	ARG ARG ARG	244 244 244 244 245 245 245 245 245 245	13 15 15 15 16 17 17 18 18 19 19 20	.038 .378 .453 .692 .916 .394 .911 .308 .429 .037 .062 .668 .429 .290 .290 .494 .949 .949 .949 .949	77.716 77.200 77.610 76.439 78.907 79.329 79.540 79.140 80.809 81.552 81.593 82.162 81.148 80.209 81.427 82.692 83.428 82.907 80.444 79.495	24.801 24.293 24.476 23.533 23.828 22.800 24.433 25.235 23.942 25.122 26.288 27.546 28.265 28.024 29.230 29.589 29.138 30.317 29.830 29.554	1.00 10.60 1.00 0.00 1.00 10.63 1.00 12.74 1.00 19.09 1.00 22.97 1.00 21.88 1.00 16.43 1.00 16.53 1.00 18.89 1.00 20.31 1.00 12.05 1.00 0.00 1.00 16.66 1.00 11.02 1.00 0.00 1.00 0.00 1.00 0.00 1.00 0.00 1.00 0.00 1.00 0.00 1.00 0.00	8888888888888888888
20 25	ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2803 2804 2805 2806 2807 2808 2809 2810	HH22 C O N H CA CB	ARG ARG ARG ARG ARG ARG ARG	245 245 246 246 246 246 246 246	20 18 19 18 17 19	0.604 3.411 9.106 3.450 7.864 9.341 9.116 9.775	80.649 80.701 79.699 81.739 82.504 81.766 83.052 83.037	30.554 22.784 22.632 21.952 22.119 20.794 19.978 18.582	1.00 0.00 1.00 13.58 1.00 14.35 1.00 16.40 1.00 0.00 1.00 16.73 1.00 20.99 1.00 27.27 1.00 29.21	8 8 8 8 8 8 8 8 8
30	ATOM ATOM ATOM ATOM ATOM ATOM	2811 2812 2813 2814 2815 2816	CD NE HE CZ NH1 HH11	ARG ARG ARG ARG ARG	246 246 246 246 246 246	20 21 20 19	9.881 0.716 1.467 0.516 9.502 3.867	81.606 81.432 80.808 82.047 82.893 83.049	18.080 16.898 16.959 15.737 15.590 16.346	1.00 29.21 1.00 40.75 1.00 0.00 1.00 40.49 1.00 44.89 1.00 0.00	B B B B
35	ATOM ATOM ATOM ATOM ATOM	2817 2818 2819	HH12	ARG ARG ARG	246 246 246 246 246	2: 2: 2: 2:	9.361 1.323 2.065 1.185 0.830	83.355 81.797 81.130 82.260 81.662	14.715 14.715 14.816 13.841 21.175	1.00 0.00 1.00 40.11 1.00 0.00 1.00 0.00 1.00 19.16	В В В В
40	ATOM ATOM ATOM ATOM ATOM	2822 2823 2824 2825 2826	O N H CA C	ARG GLY GLY GLY GLY	246 247 247 247 247	2: 2: 2: 2:	1.347 1.505 1.040 2.920 3.301	82.479 80.652 80.009 80.479 80.022	21.929 20.651 20.075 20.917 22.315	1.00 19.43 1.00 15.61 1.00 0.00 1.00 19.07 1.00 19.74	B B B B
45	MOTA MOTA ATOM ATOM MOTA	2827 2828 2829 2830 2831	O N H CA CB	GLY VAL VAL VAL VAL	247 248 248 248 248	2 2 2 2	4.479 2.320 1.390 2.619 1.466	79.869 79.793 79.916 79.361 79.725	22.618 23.170 22.891 24.528 25.475	1.00 24.75 1.00 18.96 1.00 0.00 1.00 16.15 1.00 11.70	В В В В
50	MOTA MOTA MOTA MOTA	2832 2833 2834 2835 2836	CG2 C O	VAL VAL VAL LYS	248 248 248 248 249	2 2 2	1.742 1.285 2.851 2.051 3.946	81.254 77.852 77.104 77.410	25.517 24.542 24.008 25.153	1.00 8.03 1.00 12.88 1.00 19.75 1.00 20.58 1.00 21.97	В В В В
55	ATOM ATOM ATOM ATOM ATOM	2837 2838 2839 2840 2841	H CA CB CG	LYS LYS LYS LYS	249 249 249 249 249	2 2 2	4.551 4.269 5.668 6.782 6.332	78.054 75.983 75.769 75.746 76.365	25.574 25.204 25.795 24.731 23.395	1.00 0.00 1.00 24.74 1.00 28.79 1.00 39.64 1.00 40.06	B B B B
60	MOTA MOTA MOTA MOTA	2842 2843 2844 2845 2846	CE NZ HZ1 HZ2	LYS LYS LYS LYS	249 249 249 249 249	2 2 2 2	7.485 8.289 8.706 7.672 9.047	76.507 77.759 77.775 78.587 77.784	22.393 22.567 23.518 22.444 21.855	1.00 46.49 1.00 42.34 1.00 0.00 1.00 0.00 1.00 0.00	B B B B
65	ATOM ATOM ATOM ATOM ATOM ATOM	2846 2847 2848 2849 2850 2851	C O N H	LYS LYS LYS LYS LYS	249 249 249 250 250 250	2 2 2 2	3.268 2.753 3.030 3.514 2.101	75.105 75.467 73.937 73.734	25.945 27.007 25.359 24.531 25.864	1.00 18.56 1.00 15.02 1.00 19.31 1.00 0.00 1.00 21.51	B B B B
70	ATOM ATOM ATOM ATOM	2852 2853 2854 2855	CB CG CD	LYS LYS LYS	250 250 250 250 250	2 2 2	1.440 0.819 0.380 9.318	72.228 73.146 72.344	24.684 23.641 22.404	1.00 21.98 1.00 24.29 1.00 20.75	В В В В

ATOM 2923 H GLY 258 18.302 53.127 36.277 1.00 0.00 B ATOM 2924 CA GLY 258 18.108 51.013 36.240 1.00 11.28 B ATOM 2925 C GLY 258 18.275 50.992 34.737 1.00 13.51 B ATOM 2926 O GLY 258 18.350 52.038 34.108 1.00 17.36 B ATOM 2927 N GLU 259 18.328 49.792 34.159 1.00 16.87 B										
ATOM		ΑΨΟΜ	2856	NZ LYS	250	19.629	73.074	20.143	1.00 33.42	В
ATOM 2859 H22 LYS 250						19.675	72.092	19.805	1.00 0.00	В
R-ROM   2850   H23   LYS   250   18.887   73.586   19.627   1.00   0.00   B									1.00 0.00	В
5 AROM 2860 C LYS 250 22.735 71.894 26.776 1.00 23.57 B AROM 2861 O LYS 250 23.707 71.221 26.394 1.00 20.92 B AROM 2862 N VAL 251 22.196 71.756 27.986 1.00 17.38 B AROM 2863 H VAL 251 21.459 72.339 28.260 1.00 0.00 B AROM 2864 CA VAL 251 22.708 70.748 28.899 1.00 17.18 B AROM 2866 CG1 VAL 251 23.853 70.213 31.024 1.00 6.20 B AROM 2866 CG2 VAL 251 23.853 70.213 31.024 1.00 6.20 B AROM 2866 CG2 VAL 251 23.852 70.213 31.024 1.00 6.20 B AROM 2866 CG2 VAL 251 24.542 72.269 9.833 1.00 11.43 B AROM 2866 CG2 VAL 251 24.542 72.269 9.833 1.00 11.55 B AROM 2866 CG2 VAL 251 24.542 72.269 9.833 1.00 11.55 B AROM 2866 CG2 VAL 251 24.542 72.269 9.833 1.00 11.55 B AROM 2869 O VAL 251 20.496 70.283 29.712 1.00 17.19 B AROM 2870 N MET 252 21.816 68.834 29.354 1.00 27.95 B AROM 2871 N MET 252 21.816 68.832 29.712 1.00 17.19 B AROM 2872 CA BET 252 20.851 66.658 28.570 1.00 17.19 B AROM 2873 CA BET 252 21.816 66.88 28.570 1.00 17.19 B AROM 2873 CA BET 252 21.9355 66.715 28.776 1.00 17.10 B AROM 2873 CA BET 252 19.355 66.715 28.776 1.00 17.10 B AROM 2873 CA BET 252 19.355 66.715 28.776 1.00 17.10 B AROM 2873 CA BET 252 19.355 66.715 28.776 1.00 17.10 19.80 B AROM 2875 C B MET 252 19.355 66.715 28.776 1.00 17.10 19.80 B AROM 2873 C B MET 252 21.451 66.778 30.932 1.00 17.12 B AROM 2873 C B MET 252 21.451 66.788 30.932 1.00 17.12 B AROM 2878 O MET 252 21.451 66.759 30.932 1.00 17.12 B AROM 2878 O MET 252 21.451 66.788 30.932 1.00 17.12 B AROM 2881 CA VAL 253 19.881 67.176 33.208 1.00 19.80 B AROM 2881 CA VAL 253 19.881 67.176 33.208 1.00 19.80 B AROM 2881 CA VAL 253 19.881 67.176 33.309 1.00 19.80 B AROM 2881 CA VAL 253 19.881 67.176 33.309 1.00 19.80 B AROM 2882 CB VAL 253 19.881 67.176 33.309 1.00 19.80 B AROM 2889 CB VAL 253 19.881 67.176 33.309 1.00 19.80 B AROM 2889 CB VAL 253 19.881 67.176 33.309 1.00 19.80 B AROM 2889 CB VAL 253 19.881 67.176 33.309 1.00 10.00 18.8 B AROM 2889 CB VAL 253 19.891 67.206 33.309 1.00 10.00 18.8 B AROM 2889 CB VAL 253 18.804 67.377 33.309 1.00 10.00 16.40 B AROM 2889 CB VAL 253 18.804 67.377 35.348 1									1.00 0.00	В
ATOM 2861 O LYS 250 23.707 71.221 26.394 1.00 20.922 B ATOM 2862 N VAL 251 22.198 71.756 27.986 1.00 17.38 B ATOM 2863 H VAL 251 22.198 71.756 27.986 1.00 17.38 B ATOM 2863 C VAL 251 22.708 70.748 28.899 1.00 17.18 B ATOM 2865 CG VAL 251 23.364 71.338 30.175 1.00 11.43 B ATOM 2866 CG VAL 251 23.364 71.338 30.175 1.00 11.43 B ATOM 2867 CG2 VAL 251 23.537 70.213 31.024 1.00 6.20 ATOM 2867 CG2 VAL 251 24.542 72.269 29.823 1.00 18.54 B ATOM 2867 CG2 VAL 251 21.573 69.834 29.354 1.00 18.54 B ATOM 2867 CG2 VAL 251 21.573 69.834 29.354 1.00 18.54 B ATOM 2869 O VAL 251 20.496 70.283 29.712 1.00 17.19 B ATOM 2870 N MET 252 21.831 68.537 29.332 1.00 17.99 B ATOM 2871 H MET 252 22.706 86.282 29.021 1.00 0.00 B ATOM 2873 CB MET 252 20.851 67.573 29.762 1.00 17.99 B ATOM 2873 CB MET 252 20.513 66.568 28.570 1.00 17.17 B ATOM 2873 CB MET 252 19.355 65.715 28.776 1.00 17.17 B ATOM 2873 CB MET 252 19.355 65.715 28.776 1.00 17.17 B ATOM 2873 CB MET 252 19.355 66.746 27.476 1.00 17.17 B ATOM 2873 CB MET 252 19.355 66.715 28.776 1.00 17.19 B ATOM 2875 CB MET 252 19.355 66.715 28.776 1.00 17.10 B ATOM 2875 CB MET 252 19.355 66.715 28.776 1.00 17.10 B ATOM 2875 CB MET 252 19.355 66.715 28.776 1.00 17.10 B ATOM 2875 CB MET 252 19.355 66.715 28.076 1.00 17.10 B ATOM 2875 CB MET 252 19.355 66.715 28.076 1.00 17.10 B ATOM 2875 CB MET 252 19.355 66.715 28.076 1.00 17.10 B ATOM 2875 CB MET 252 19.355 66.715 28.076 1.00 17.10 B ATOM 2875 CB MET 252 19.355 66.715 28.076 1.00 17.10 B ATOM 2875 CB MET 252 19.355 66.715 28.076 1.00 17.10 B ATOM 2875 CB MET 252 19.355 66.715 28.076 1.00 17.10 B ATOM 2875 CB MET 252 19.355 66.715 28.076 1.00 17.10 B ATOM 2875 CB MET 252 19.355 66.715 28.077 1.00 17.10 B ATOM 2875 CB MET 252 19.355 66.715 28.077 1.00 17.10 B ATOM 2875 CB MET 252 19.355 66.715 28.077 1.00 17.10 B ATOM 2875 CB MET 252 19.355 66.715 28.077 1.00 17.10 B ATOM 2875 CB MET 252 29.22 24.618 66.777 30.922 1.00 15.72 B ATOM 2875 CB MET 252 29.22 24.618 66.777 30.922 1.00 15.72 B ATOM 2875 CB MET 252 29.22 29.22 29.22 29.22 29.22 29.22 29.	5									
MOOM   2865   N   VAL   251   22.198   71.756   27.986   1.00   17.38   B   ROM   2864   CA   VAL   251   21.459   72.399   28.260   1.00   0.00   0.00   28.260   1.00   28.260   1.00   17.18   B   28.260   1.00   17.18   B   28.260   1.00   28.260   1.00   17.18   B   28.260   1.00   17.20   28.260   1.00   11.43   B   28.260   11.00   11.43   B   28.260   11.00   11.43   B   28.260   11.00   11.00   11.43   B   28.260   11.00   11.13   B   28.260   11.20   11.00   11.13   B   28.260   11.20   11.00   11.13   B   28.260   11.20   11.20   11.20   B   28.260   11.20   11.20   B   28.260   11.20   11.20   11.20   B   28.260   11.20   11.20   B   28.260   11.20   11.20   11.20   B   28.260   11.20	5									
NOON										
MOM										
10										
APTOM   2866   CGI   VAL   251   23.853   70.213   31.024   1.00   6.20   8   APTOM   2867   CGI   VAL   251   24.542   72.269   29.823   1.00   18.548   8   APTOM   2868   C   VAL   251   20.496   70.283   29.712   1.00   10.955   8   APTOM   2870   N   MET   252   21.831   68.537   29.332   1.00   17.99   8   APTOM   2871   M   MET   252   20.851   67.573   29.762   1.00   18.29   8   APTOM   2872   CA   MET   252   20.851   67.573   29.762   1.00   18.29   8   APTOM   2873   CR   MET   252   20.851   67.573   29.762   1.00   18.29   8   APTOM   2874   CG   MET   252   20.851   67.573   29.762   1.00   18.29   8   APTOM   2875   CG   MET   252   20.851   67.573   29.762   1.00   18.29   8   APTOM   2875   CG   MET   252   20.851   67.573   29.762   1.00   19.60   8   APTOM   2876   CG   MET   252   19.355   65.715   28.776   1.00   17.10   P. 60   APTOM   2876   CG   MET   252   19.355   65.715   28.776   1.00   17.10   P. 60   APTOM   2878   CG   MET   252   19.355   65.715   28.776   1.00   17.10   P. 60   P. ATOM   2879   N   VAL   253   20.731   66.666   23.048   1.00   18.09   B. ATOM   2879   N   VAL   253   20.731   66.666   23.048   1.00   18.09   B. ATOM   2881   CA   VAL   253   21.261   66.778   30.932   1.00   17.72   B. ATOM   2881   CA   VAL   253   21.261   66.788   34.863   1.00   17.42   B. ATOM   2884   CG   VAL   253   21.261   66.788   34.863   1.00   17.42   B. ATOM   2884   CG   VAL   253   21.261   66.788   34.863   1.00   17.42   B. ATOM   2885   CG   VAL   253   21.261   66.788   34.863   1.00   16.44   B. ATOM   2886   CG   VAL   253   21.261   66.788   34.863   1.00   16.44   B. ATOM   2886   CG   VAL   253   20.161   67.266   33.208   1.00   10.04   4.498   B. ATOM   2888   CG   VAL   253   20.161   67.266   33.208   1.00   10.04   B. ATOM   2888   CG   VAL   253   20.161   67.266   33.208   1.00   10.04   4.498   B. ATOM   2889   CG   VAL   253   20.161   67.266   33.208   1.00   20.30   B. ATOM   2898   CG   VAL   253   20.161   67.266   33.208   1.00   20.30   B. ATOM   2899	10									
ATOM 2867 COZ VAL 251 22.5.12.5.73 69.834 29.354 1.00 18.54 B ATOM 2868 C VAL 251 21.573 69.834 29.354 1.00 12.95 B ATOM 2870 N MET 252 21.831 68.537 29.332 1.00 17.99 B ATOM 2870 N MET 252 21.831 68.537 29.332 1.00 17.99 B ATOM 2871 N MET 252 21.831 68.537 29.332 1.00 17.99 B ATOM 2873 CA MET 252 20.551 67.573 29.762 1.00 17.99 B ATOM 2873 CA MET 252 20.551 67.573 29.762 1.00 17.87 B ATOM 2874 CA MET 252 20.551 67.573 29.762 1.00 17.87 B ATOM 2874 CA MET 252 20.551 67.573 29.762 1.00 17.87 B ATOM 2874 CA MET 252 20.551 67.573 29.762 1.00 17.87 B ATOM 2875 SD MET 252 19.057 64.546 27.405 1.00 15.69 B ATOM 2875 CA MET 252 19.057 64.546 27.405 1.00 15.69 B ATOM 2876 CA MET 252 19.057 64.546 27.405 1.00 15.72 B ATOM 2878 CA MET 252 21.612 66.778 30.932 1.00 15.72 B ATOM 2878 O MET 252 21.651 66.778 30.932 1.00 15.72 B ATOM 2878 O MET 252 21.666 66.280 30.827 1.00 19.70 G B ATOM 2878 O MET 252 21.666 66.280 30.827 1.00 19.70 G B ATOM 2881 CA VAL 253 19.881 67.176 32.096 1.00 0.00 B ATOM 2882 CA VAL 253 19.881 67.176 32.096 1.00 0.00 D B ATOM 2882 CA VAL 253 12.101 66.788 34.496 1.00 16.44 B ATOM 2884 CA VAL 253 19.881 67.176 32.096 1.00 10.00 J B ATOM 2884 CA VAL 253 19.881 67.176 33.098 1.00 17.72 B ATOM 2884 N M M M M M M M M M M M M M M M M M M	10									
APTOM   2868   C   VAL   251   21.573   69.834   29.354   1.00   20.95   B										
APPEN   2889   O VAL   251   20.496   70.283   29.712   1.00   17.19   B										
15										
ATOM 2871 H MET 252 22.706 68.228 29.021 1.00 0.00 0.00 ATOM 2872 CA MET 252 20.851 67.573 29.762 1.00 18.29 B ATOM 2873 CB MET 252 20.513 66.658 28.570 1.00 17.87 B ATOM 2874 CG MET 252 19.057 64.546 27.405 1.00 35.69 B ATOM 2875 CB MET 252 19.057 64.546 27.405 1.00 35.69 B ATOM 2877 C MET 252 19.057 64.546 27.405 1.00 35.69 B ATOM 2877 C MET 252 19.057 64.546 27.405 1.00 35.69 B ATOM 2877 C MET 252 19.057 64.546 27.405 1.00 17.71 B ATOM 2877 C MET 252 21.451 66.778 30.932 1.00 19.60 B ATOM 2878 D MET 252 21.451 66.778 30.932 1.00 19.38 B ATOM 2879 N VAL 253 19.81 67.716 32.096 1.00 0.00 B ATOM 2881 CA VAL 253 19.81 67.716 32.096 1.00 0.00 B ATOM 2881 CA VAL 253 19.81 67.716 32.096 1.00 0.00 B ATOM 2882 CB VAL 253 20.21 1.65 65.916 33.208 1.00 17.72 B ATOM 2883 CGI VAL 253 20.61 68.051 34.263 1.00 9.88 B ATOM 2885 CB VAL 253 20.61 68.051 34.263 1.00 9.88 B ATOM 2885 CB VAL 253 39.80 67.50 1.51 64.756 33.379 1.00 20.14 B ATOM 2885 CB VAL 253 39.80 67.50 1.51 64.756 33.379 1.00 20.14 B ATOM 2885 CB VAL 253 30.51 64.756 33.379 1.00 20.14 B ATOM 2885 CB VAL 253 19.91 64.756 33.379 1.00 20.14 B ATOM 2885 CB VAL 253 19.91 64.756 33.379 1.00 20.14 B ATOM 2885 CB VAL 253 19.91 64.756 33.379 1.00 20.14 B ATOM 2885 CB VAL 253 19.91 64.756 33.379 1.00 20.14 B ATOM 2885 CB VAL 253 19.91 64.756 33.379 1.00 20.14 B ATOM 2885 CB VAL 253 19.91 64.756 33.379 1.00 20.14 B ATOM 2889 CB LIE 254 19.915 62.360 33.335 1.00 24.01 B ATOM 2889 CB LIE 254 19.915 62.360 33.335 1.00 24.01 B ATOM 2889 CB LIE 254 19.915 62.360 33.335 1.00 24.01 B ATOM 2889 CB LIE 254 19.915 62.360 33.335 1.00 24.01 B ATOM 2893 CDI LIE 254 19.915 62.360 33.335 1.00 24.01 B ATOM 2899 CB VAL 255 19.916 60.92 69.21 1.83 1.00 24.01 B ATOM 2899 CB VAL 255 19.916 60.92 69.21 1.00 16.06 B ATOM 2899 CB VAL 255 19.916 60.92 69.21 1.00 16.06 B ATOM 2899 CB VAL 255 19.916 60.92 69.21 1.00 16.06 B ATOM 2899 CB VAL 255 19.916 60.92 69.21 1.00 16.15 B ATOM 2900 CG VAL 255 19.916 60.92 69.31 1.00 10.00 10.00 B ATOM 2900 CG VAL 255 19.916 60.92 60.92 1.00 16.15 B ATOM 2900	1.5									
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ATOM 2884 CG2 VAL 253 19.802 67.226 34.861 1.00 28.03 B ATOM 2886 C VAL 253 20.151 64.756 33.379 1.00 20.14 B ATOM 2887 N ILE 254 20.607 63.517 33.226 1.00 24.01 B ATOM 2888 H ILE 254 21.557 63.374 33.638 1.00 18.38 B ATOM 2889 CA ILE 254 19.715 62.360 33.335 1.00 20.30 B ATOM 2899 CB ILE 254 19.903 61.386 32.137 1.00 24.38 B ATOM 2891 CG2 ILE 254 19.903 61.386 32.137 1.00 24.38 B ATOM 2892 CG1 ILE 254 19.903 61.386 32.137 1.00 24.38 B ATOM 2895 CD1 ILE 254 19.903 61.386 32.137 1.00 24.38 B ATOM 2895 CD1 ILE 254 19.913 61.360 32.183 1.00 21.87 B ATOM 2895 CD1 ILE 254 19.914 61.596 34.635 1.00 26.33 B ATOM 2896 N VAL 255 18.804 61.377 35.348 1.00 16.92 B ATOM 2897 N VAL 255 18.804 61.377 35.348 1.00 16.92 B ATOM 2899 CB VAL 255 18.804 61.377 35.348 1.00 16.92 B ATOM 2899 CB VAL 255 18.796 60.692 36.629 1.00 16.15 B ATOM 2899 CC VAL 255 18.796 60.692 36.629 1.00 16.15 B ATOM 2900 CG1 VAL 255 18.178 61.580 37.725 1.00 18.84 B ATOM 2901 CG2 VAL 255 18.215 60.856 39.071 1.00 10.30 B ATOM 2904 N THR 256 18.584 58.301 36.811 1.00 13.71 B ATOM 2906 CA THR 256 19.507 59.480 36.629 1.00 16.40 B ATOM 2907 CB THR 256 19.507 59.348 36.484 1.00 13.71 B ATOM 2908 OG1 THR 256 19.507 58.326 37.105 1.00 10.778 B ATOM 2909 HG1 THR 256 19.507 58.326 37.105 1.00 10.30 B ATOM 2909 HG1 THR 256 19.507 58.326 37.105 1.00 10.31 B ATOM 2909 HG1 THR 256 19.507 58.326 37.105 1.00 10.775 B ATOM 2909 TO THR 256 19.507 58.326 37.105 1.00 10.775 B ATOM 2901 CG2 THR 256 19.507 58.326 37.105 1.00 10.775 B ATOM 2911 C THR 256 18.542 55.359 35.006 1.00 15.12 B ATOM 2913 N ASP 257 17.799 54.348 37.881 1.00 15.42 B ATOM 2914 H ASP 257 17.799 54.948 37.881 1.00 15.42 B ATOM 2915 CA ASP 257 18.198 53.872 38.745 1.00 18.63 B ATOM 2917 CG ASP 257 17.481 53.974 40.119 1.00 17.76 B ATOM 2919 OD2 ASP 257 17.481 53.974 40.119 1.00 17.76 B ATOM 2910 OD ASP 257 17.892 53.127 37.553 1.00 18.63 B ATOM 2910 OD ASP 257 17.892 53.127 37.553 1.00 18.63 B ATOM 2910 OD ASP 257 17.892 53.127 37.553 1.00 18.63 B ATOM 2910 OD ASP 257 17.892 53.127 38.217 1.00 10.655 B A		MOTA	2882							
ATOM 2885 C VAL 253 20.151 64.756 33.379 1.00 20.14 B ATOM 2887 N ILE 254 20.507 63.517 33.226 1.00 24.01 B ATOM 2887 N ILE 254 20.507 63.517 33.226 1.00 24.01 B ATOM 2888 H ILE 254 20.507 63.517 33.226 1.00 24.01 B ATOM 2888 H ILE 254 21.557 63.374 33.037 1.00 20.30 B ATOM 2889 CA ILE 254 19.715 62.360 33.335 1.00 20.30 B ATOM 2890 CB ILE 254 19.715 62.360 33.335 1.00 20.30 B ATOM 2891 CG2 ILE 254 19.903 61.386 32.137 1.00 24.38 B ATOM 2892 CG1 ILE 254 19.916 62.360 32.183 1.00 21.87 B ATOM 2893 CD1 ILE 254 19.916 62.500 30.176 1.00 26.33 B ATOM 2895 C ILE 254 19.916 61.590 34.635 1.00 21.87 B ATOM 2895 C ILE 254 21.107 62.500 30.176 1.00 26.33 B ATOM 2895 C ILE 254 21.007 62.500 30.176 1.00 21.12 B ATOM 2898 CA VAL 255 18.804 61.377 35.348 1.00 21.12 B ATOM 2898 CA VAL 255 18.804 61.377 35.348 1.00 16.92 B ATOM 2899 CB VAL 255 18.804 61.377 35.348 1.00 16.92 B ATOM 2899 CA VAL 255 18.906 60.692 36.629 1.00 16.15 B ATOM 2900 CG1 VAL 255 18.18 61.580 37.725 1.00 18.84 B ATOM 2900 CG1 VAL 255 18.216 60.856 39.071 1.00 10.30 B ATOM 2900 CG1 VAL 255 18.916 60.856 39.071 1.00 10.30 B ATOM 2901 CG2 VAL 255 18.916 60.856 39.071 1.00 10.30 B ATOM 2902 C VAL 255 17.970 59.434 36.484 1.00 15.00 B ATOM 2904 N THR 256 18.584 58.301 36.781 1.00 16.46 B ATOM 2909 CB THR 256 18.584 58.301 36.781 1.00 16.40 B ATOM 2909 CC VAL 255 17.990 59.480 36.109 1.00 16.40 B ATOM 2909 CC THR 256 18.584 58.301 36.781 1.00 14.62 B ATOM 2909 CC THR 256 17.960 57.022 36.634 1.00 15.00 B ATOM 2909 CC THR 256 18.584 58.301 36.781 1.00 16.46 B ATOM 2909 CC THR 256 18.584 58.301 36.781 1.00 17.78 B ATOM 2901 CG2 THR 256 17.960 57.022 36.634 1.00 15.00 B ATOM 2909 CC THR 256 17.960 57.022 36.634 1.00 15.00 B ATOM 2909 CC THR 256 17.960 57.022 36.634 1.00 15.00 B ATOM 2909 CC THR 256 17.960 57.022 36.634 1.00 15.00 B ATOM 2909 CC THR 256 17.960 57.022 36.634 1.00 15.00 B ATOM 2909 CC THR 256 18.594 58.301 36.781 1.00 16.63 B ATOM 2910 CC THR 256 18.594 59.595 37.006 1.00 10.00 16.43 B ATOM 2910 CC THR 256 18.595 18.935 38.301 36.029 1.00 16.31 B A		MOTA	2883	CG1 VAL						
ATOM 2886 O VAL 253 18.974 64.981 33.648 1.00 18.38 B ATOM 2887 N ILE 254 20.607 63.517 33.226 1.00 24.01 B ATOM 2888 H ILE 254 21.557 63.573 33.237 1.00 0.00 B ATOM 2889 CA ILE 254 19.715 62.360 33.335 1.00 20.30 B ATOM 2890 CB ILE 254 19.903 61.386 32.137 1.00 20.30 B ATOM 2891 CG2 ILE 254 19.903 61.386 32.137 1.00 21.87 B ATOM 2892 CG1 ILE 254 19.784 62.147 30.816 1.00 21.87 B ATOM 2893 CD1 ILE 254 19.784 62.147 30.816 1.00 21.87 B ATOM 2893 CD1 ILE 254 19.784 62.147 30.816 1.00 21.87 B ATOM 2894 C ILE 254 19.911 61.596 34.635 1.00 21.12 B ATOM 2895 O ILE 254 21.107 62.500 30.176 1.00 26.33 B ATOM 2896 N VAL 255 18.804 61.377 35.348 1.00 21.12 B ATOM 2897 H VAL 255 17.951 61.700 34.986 1.00 0.00 B ATOM 2898 CA VAL 255 18.804 61.377 35.348 1.00 21.12 B ATOM 2899 CB VAL 255 18.178 61.580 37.725 1.00 16.15 B ATOM 2900 CG1 VAL 255 18.178 61.580 37.725 1.00 16.15 B ATOM 2901 CG2 VAL 255 18.178 61.580 37.725 1.00 16.15 B ATOM 2900 CG1 VAL 255 18.178 61.580 37.725 1.00 16.03 B ATOM 2901 CG2 VAL 255 18.178 61.580 37.725 1.00 16.06 B ATOM 2904 N THR 256 18.594 59.480 36.109 1.00 16.40 B ATOM 2905 H THR 256 19.507 59.434 36.434 1.00 13.71 B ATOM 2906 CA THR 256 19.507 58.326 37.105 1.00 0.00 B ATOM 2909 HG1 THR 256 19.507 58.326 37.105 1.00 0.00 B ATOM 2909 HG1 THR 256 19.507 58.326 37.105 1.00 0.00 B ATOM 2901 CG2 THR 256 19.444 56.327 34.704 1.00 17.78 B ATOM 2910 CG2 THR 256 19.444 56.327 34.704 1.00 10.75 B ATOM 2911 C THR 256 19.507 58.326 37.105 1.00 0.00 B ATOM 2911 C THR 256 19.444 56.327 34.704 1.00 10.75 B ATOM 2911 C THR 256 19.445 56.327 34.704 1.00 10.75 B ATOM 2910 CG2 THR 256 19.445 56.327 34.704 1.00 10.75 B ATOM 2911 C THR 256 19.449 56.327 34.704 1.00 10.75 B ATOM 2911 C THR 256 19.507 58.326 37.105 1.00 0.00 B ATOM 2913 N ASP 257 17.739 54.948 37.531 1.00 16.63 B ATOM 2913 N ASP 257 17.739 54.948 37.533 1.00 0.00 B ATOM 2914 H ASP 257 15.892 52.706 41.219 1.00 16.43 B ATOM 2915 CA ASP 257 15.892 52.706 41.219 1.00 17.76 B ATOM 2915 CA ASP 257 15.892 52.706 41.219 1.00 16.63 B ATOM 2921 C ASP 257 15.		MOTA	2884	CG2 VAL						
ATOM 2887 N ILE 254 20.607 63.517 33.226 1.00 24.01 B ATOM 2888 H ILE 254 21.557 63.374 33.037 1.00 0.00 B ATOM 2889 CA ILE 254 19.715 62.360 33.335 1.00 20.30 B ATOM 2890 CB ILE 254 19.903 61.386 32.137 1.00 24.38 B ATOM 2891 CG2 ILE 254 18.849 60.290 32.183 1.00 21.87 B ATOM 2892 CG1 ILE 254 19.903 61.386 32.137 1.00 24.38 B ATOM 2893 CD1 ILE 254 21.107 62.500 30.176 1.00 26.33 B ATOM 2893 CD1 ILE 254 21.107 62.500 30.176 1.00 26.33 B ATOM 2894 C ILE 254 19.911 61.596 34.635 1.00 21.12 B ATOM 2895 D ILE 254 21.107 62.500 34.777 35.348 1.00 16.92 B ATOM 2897 H VAL 255 18.804 61.377 35.348 1.00 16.92 B ATOM 2897 H VAL 255 17.951 61.700 34.986 1.00 18.90 B ATOM 2899 CB VAL 255 18.796 60.692 36.629 1.00 16.15 B ATOM 2900 CG1 VAL 255 18.178 61.580 37.725 1.00 18.84 B ATOM 2901 CG2 VAL 255 18.178 61.580 37.725 1.00 18.84 B ATOM 2901 CG2 VAL 255 18.315 60.856 39.071 1.00 10.30 B ATOM 2903 O VAL 255 18.916 60.892 37.706 1.00 10.30 B ATOM 2903 O VAL 255 18.916 60.892 37.706 1.00 10.30 B ATOM 2903 O VAL 255 18.913 62.925 37.706 1.00 10.30 B ATOM 2903 O VAL 255 18.913 62.925 37.706 1.00 10.30 B ATOM 2904 N THR 256 18.584 58.301 36.781 1.00 14.62 B ATOM 2905 C VAL 255 18.915 60.856 39.071 1.00 10.30 B ATOM 2905 C VAL 255 18.915 60.895 37.105 1.00 16.06 B ATOM 2909 HG1 THR 256 17.906 57.022 36.634 1.00 13.71 B ATOM 2909 HG1 THR 256 17.906 57.022 36.634 1.00 13.71 B ATOM 2909 HG1 THR 256 17.906 57.022 36.634 1.00 17.78 B ATOM 2910 CG2 VAL 255 18.915 55.359 37.105 1.00 16.43 B ATOM 2911 C THR 256 19.507 58.326 37.105 1.00 16.43 B ATOM 2911 C THR 256 19.507 58.326 37.105 1.00 16.43 B ATOM 2912 C A SP 257 18.815 54.937 37.555 1.00 18.63 B ATOM 2910 CG2 THR 256 19.507 58.326 37.105 1.00 16.53 B ATOM 2911 C THR 256 19.507 58.326 37.105 1.00 16.53 B ATOM 2912 C A SP 257 18.615 53.937 37.555 1.00 16.53 B ATOM 2913 N ASP 257 17.739 59.434 38.7881 1.00 16.63 B ATOM 2913 N ASP 257 17.739 59.434 34.737 1.00 16.53 B ATOM 2912 C A SP 257 18.667 52.456 38.158 1.00 15.10 B ATOM 2912 C A SP 257 18.667 52.456 38.158 1.00 15.10 B ATOM 2912	30	MOTA	2885	C VAL						
ATOM 2888 H ILE 254 21.557 63.374 33.037 1.00 0.00 B ATOM 2889 CA ILE 254 19.715 62.360 33.335 1.00 20.30 B ATOM 2889 CB ILE 254 19.903 61.386 32.137 1.00 24.38 B ATOM 2891 CG2 ILE 254 19.903 61.386 32.137 1.00 24.38 B ATOM 2892 CG1 ILE 254 19.784 62.147 30.816 1.00 21.87 B ATOM 2893 CD1 ILE 254 19.784 62.147 30.816 1.00 21.87 B ATOM 2893 CD1 ILE 254 19.784 62.147 30.816 1.00 21.87 B ATOM 2894 C ILE 254 19.784 62.147 30.816 1.00 26.33 B ATOM 2895 O ILE 254 21.017 62.500 30.176 1.00 26.33 B ATOM 2895 N VAL 255 18.804 61.576 34.635 1.00 21.12 B ATOM 2897 H VAL 255 17.951 61.596 34.635 1.00 16.92 B ATOM 2897 H VAL 255 18.804 61.377 35.348 1.00 16.92 B ATOM 2899 CB VAL 255 18.786 60.692 36.629 1.00 16.15 B ATOM 2890 CG1 VAL 255 18.178 61.580 37.725 1.00 18.84 B ATOM 2900 CG1 VAL 255 18.178 61.580 37.725 1.00 18.84 B ATOM 2900 CG1 VAL 255 18.215 60.856 37.725 1.00 16.05 B ATOM 2900 CG1 VAL 255 18.931 62.925 37.796 1.00 16.06 B ATOM 2903 O VAL 255 18.78 61.580 37.775 1.00 16.06 B ATOM 2904 N THR 256 18.584 58.301 36.781 1.00 10.30 B ATOM 2904 N THR 256 18.584 58.301 36.781 1.00 14.62 B ATOM 2907 CB THR 256 17.970 59.480 36.109 1.00 16.40 B ATOM 2907 CB THR 256 17.950 56.564 35.161 1.00 17.78 B ATOM 2909 HG1 THR 256 17.950 57.022 36.634 1.00 17.78 B ATOM 2909 HG1 THR 256 17.950 56.564 35.161 1.00 17.78 B ATOM 2909 HG1 THR 256 17.950 56.564 35.161 1.00 17.78 B ATOM 2911 C THR 256 17.950 56.564 37.523 1.00 16.31 B ATOM 2911 C THR 256 17.950 56.564 37.523 1.00 16.31 B ATOM 2912 O THR 256 17.950 56.564 37.523 1.00 16.31 B ATOM 2911 C THR 256 17.950 56.564 37.523 1.00 16.31 B ATOM 2911 C THR 256 17.950 56.564 37.523 1.00 16.31 B ATOM 2911 C THR 256 17.950 56.564 37.523 1.00 16.31 B ATOM 2911 C AND 2912 C AND 2913 NASP 257 16.815 54.937 37.553 1.00 16.31 B ATOM 2914 C AND 2915 CA AND 2915 CA BASP 257 17.739 59.484 37.881 1.00 17.76 B ATOM 2910 CG2 THR 256 17.965 53.241 40.153 1.00 16.53 B ATOM 2919 OD2 AND 257 16.815 54.937 37.553 1.00 0.00 B B ATOM 2917 C AND 2918 C AN		MOTA	2886	O VAL	253					
ATOM 2889 CA ILE 254 19.715 62.360 33.335 1.00 20.30 B ATOM 2890 CB ILE 254 19.903 61.386 32.137 1.00 24.38 B ATOM 2891 CG2 ILE 254 18.849 60.290 32.183 1.00 21.87 B ATOM 2893 CD1 ILE 254 19.784 62.147 30.816 1.00 20.74 B ATOM 2893 CD1 ILE 254 21.107 62.500 30.176 1.00 26.33 B ATOM 2894 C ILE 254 21.017 62.500 30.176 1.00 26.33 B ATOM 2895 O ILE 254 21.017 62.500 30.176 1.00 26.33 B ATOM 2896 N VAL 255 18.804 61.317 35.348 1.00 21.12 B ATOM 2897 H VAL 255 18.804 61.317 35.348 1.00 16.92 B ATOM 2898 CA VAL 255 18.916 61.700 34.986 1.00 10.00 B ATOM 2898 CA VAL 255 18.916 61.700 34.986 1.00 16.15 B ATOM 2899 CB VAL 255 18.178 61.580 37.725 1.00 18.84 B ATOM 2900 CG1 VAL 255 18.215 60.856 39.071 1.00 10.30 B ATOM 2901 CG2 VAL 255 18.913 62.255 37.796 1.00 16.06 B ATOM 2903 O VAL 255 18.931 62.255 37.796 1.00 16.06 B ATOM 2904 N THR 256 18.584 58.301 36.781 1.00 14.62 B ATOM 2905 CB THR 256 19.507 58.326 37.105 1.00 16.40 B ATOM 2907 CB THR 256 19.507 58.326 37.105 1.00 15.00 B ATOM 2908 OG1 THR 256 17.950 56.564 35.161 1.00 15.00 B ATOM 2909 HG1 THR 256 17.950 56.564 35.161 1.00 15.00 B ATOM 2909 HG1 THR 256 17.950 56.564 35.161 1.00 15.00 B ATOM 2909 HG1 THR 256 17.950 56.564 35.161 1.00 15.00 B ATOM 2909 HG1 THR 256 17.950 56.564 35.161 1.00 17.78 B ATOM 2911 C THR 256 19.414 56.327 34.704 1.00 15.00 B ATOM 2911 C THR 256 18.542 55.557 35.259 1.00 0.00 B ATOM 2911 C THR 256 19.414 56.327 34.704 1.00 16.43 B ATOM 2914 H ASP 257 16.815 54.937 37.553 1.00 16.43 B ATOM 2915 CA ASP 257 16.815 54.937 37.553 1.00 16.43 B ATOM 2916 CB ASP 257 16.815 53.241 40.153 1.00 16.65 B ATOM 2917 CG ASP 257 15.492 53.317 39.107 1.00 16.65 B ATOM 2918 OD ASP 257 15.492 53.317 39.107 1.00 16.65 B ATOM 2919 OD ASP 257 15.492 53.317 39.107 1.00 16.65 B ATOM 2910 CC ASP 257 15.492 53.317 39.107 1.00 16.65 B ATOM 2910 C ASP 257 15.492 53.317 39.107 1.00 16.65 B ATOM 2921 C ASP 257 15.492 53.317 39.107 1.00 16.65 B ATOM 2922 N GLY 258 18.108 51.013 36.240 1.00 17.76 B ATOM 2923 N GLY 258 18.108 51.013 36.240 1.00 17.76 B ATOM 2925 C GLY		ATOM	2887	N ILE	254					
ATOM   2890   CB   TILE   254   19.903   61.386   32.137   1.00   24.38   B   ATOM   2891   CG2   TILE   254   18.849   60.290   32.183   1.00   21.87   B   ATOM   2892   CG1   TILE   254   19.914   62.147   30.816   1.00   20.74   B   ATOM   2893   CD1   TILE   254   21.107   62.500   30.176   1.00   26.33   B   ATOM   2895   O TILE   254   21.107   62.500   30.176   1.00   26.33   B   ATOM   2895   O TILE   254   21.107   62.500   30.176   1.00   26.33   B   ATOM   2896   N VAL   255   T1.951   61.215   34.976   1.00   18.90   B   ATOM   2897   N VAL   255   T1.951   61.215   34.976   1.00   18.90   B   ATOM   2898   CA   VAL   255   T1.951   61.270   34.986   1.00   0.00   B   ATOM   2899   CB   VAL   255   T1.951   61.700   34.986   1.00   0.00   B   ATOM   2899   CG   VAL   255   T1.951   61.580   37.725   1.00   16.15   B   ATOM   2900   CG1   VAL   255   T1.951   61.580   37.725   1.00   16.15   B   ATOM   2901   CG2   VAL   255   T1.970   59.434   36.484   1.00   13.71   B   ATOM   2902   C   VAL   255   T1.970   59.434   36.484   1.00   13.71   B   ATOM   2904   N   THR   256   T1.970   59.434   36.484   1.00   13.71   B   ATOM   2905   CB   THR   256   T1.950   56.564   35.161   1.00   14.62   B   ATOM   2907   CB   THR   256   T1.950   56.564   35.161   1.00   17.78   B   ATOM   2908   CG1   THR   256   T1.966   55.359   35.006   1.00   23.15   B   ATOM   2909   CG1   THR   256   T1.966   55.359   35.006   1.00   23.15   B   ATOM   2910   CG2   THR   256   T1.966   55.359   35.006   1.00   23.15   B   ATOM   2910   CG2   THR   256   T1.966   55.359   35.006   1.00   23.15   B   ATOM   2911   C   THR   256   T1.966   55.359   35.006   1.00   23.15   B   ATOM   2911   C   THR   256   T1.966   55.359   35.006   1.00   23.15   B   ATOM   2911   C   THR   256   T1.966   55.359   35.006   1.00   23.15   B   ATOM   2912   C   ASP   257   T1.787   54.94   53.77   35.359   1.00   10.06   B   ATOM   2913   N   ASP   257   T1.866   55.359   37.961   1.00   16.43   B   ATOM   2914   CA   ASP   257   T1.866   5		MOTA	2888	H ILE	254	21.557				
ATOM 2891 CG2 ILE 254 18.849 60.290 32.183 1.00 21.87 B ATOM 2892 CG1 ILE 254 19.784 62.147 30.816 1.00 20.74 BTOM 2893 CD1 ILE 254 21.107 62.500 30.176 1.00 26.33 B ATOM 2894 C ILE 254 21.107 62.500 30.176 1.00 26.33 B ATOM 2895 O ILE 254 21.031 61.596 34.635 1.00 21.12 B ATOM 2896 N VAL 255 18.804 61.377 35.348 1.00 16.92 B ATOM 2897 H VAL 255 17.951 61.700 34.986 1.00 16.92 B ATOM 2898 CA VAL 255 18.796 60.692 36.629 1.00 16.15 B ATOM 2899 CB VAL 255 18.796 60.692 36.629 1.00 16.15 B ATOM 2900 CG1 VAL 255 18.215 60.856 39.071 1.00 18.84 B ATOM 2901 CG2 VAL 255 18.913 62.255 37.776 1.00 18.84 B ATOM 2903 O VAL 255 18.913 62.255 37.776 1.00 16.06 B ATOM 2903 O VAL 255 16.799 59.480 36.109 1.00 16.06 B ATOM 2904 N THR 256 18.584 58.301 36.781 1.00 14.62 B ATOM 2905 H THR 256 19.507 58.326 37.105 1.00 14.62 B ATOM 2907 CB THR 256 17.950 56.564 35.161 1.00 14.62 B ATOM 2909 HG1 THR 256 17.950 56.564 35.161 1.00 17.78 B ATOM 2909 HG1 THR 256 17.950 56.564 37.105 1.00 0.00 B ATOM 2909 HG1 THR 256 17.950 56.564 37.105 1.00 0.00 B ATOM 2901 CG2 THR 256 17.950 56.564 37.105 1.00 10.75 B ATOM 2901 CG2 THR 256 17.950 56.564 37.105 1.00 0.00 B ATOM 2909 HG1 THR 256 17.950 56.564 37.105 1.00 0.00 B ATOM 2909 HG1 THR 256 17.950 56.564 37.105 1.00 0.00 B ATOM 2909 HG1 THR 256 17.950 56.564 37.105 1.00 0.00 B ATOM 2909 GC2 THR 256 19.507 58.326 37.105 1.00 0.00 B ATOM 2910 CG2 THR 256 19.414 56.327 34.704 1.00 10.75 B ATOM 2910 CG2 THR 256 19.414 56.327 34.704 1.00 10.75 B ATOM 2911 C THR 256 19.414 56.327 34.704 1.00 10.75 B ATOM 2912 O THR 256 19.414 56.327 34.704 1.00 10.75 B ATOM 2913 N ASP 257 17.739 54.948 37.821 1.00 16.43 B ATOM 2914 H ASP 257 15.782 52.706 41.219 1.00 16.63 B ATOM 2915 CA ASP 257 17.872 51.478 88.892 1.00 17.76 B ATOM 2916 CB ASP 257 17.872 51.478 88.892 1.00 17.76 B ATOM 2918 ODL ASP 257 17.872 51.478 88.892 1.00 17.76 B ATOM 2921 O ASP 257 17.872 51.478 88.892 1.00 17.76 B ATOM 2922 N GLY 258 18.108 51.013 36.240 1.00 11.28 B ATOM 2923 H GLY 258 18.108 51.013 36.240 1.00 11.28 B ATOM 2924 CA GLY 2		ATOM	2889	CA ILE	254	19.715				
ATOM 2893 CGI ILE 254 19.784 62.147 30.816 1.00 20.74 B ATOM 2893 CDI ILE 254 19.911 61.596 34.635 1.00 21.12 B ATOM 2894 C ILE 254 19.911 61.596 34.635 1.00 21.12 B ATOM 2895 O ILE 254 21.031 61.215 34.976 1.00 18.90 B ATOM 2896 N VAL 255 17.951 61.700 34.986 1.00 16.92 B ATOM 2897 H VAL 255 17.951 61.700 34.986 1.00 0.00 B ATOM 2898 CA VAL 255 18.796 60.692 36.629 1.00 16.15 B ATOM 2899 CB VAL 255 18.796 60.692 36.629 1.00 16.15 B ATOM 2900 CGI VAL 255 18.796 60.692 36.629 1.00 16.15 B ATOM 2901 CG2 VAL 255 18.795 60.856 39.071 1.00 13.03 B ATOM 2901 CG2 VAL 255 18.215 60.856 39.071 1.00 13.03 B ATOM 2901 CG2 VAL 255 18.931 62.925 37.796 1.00 16.06 B ATOM 2902 C VAL 255 17.970 59.434 36.484 1.00 13.71 B ATOM 2904 N THR 256 18.584 58.301 36.781 1.00 14.62 B ATOM 2905 H THR 256 19.507 58.326 37.105 1.00 10.462 B ATOM 2907 CB THR 256 17.906 57.022 36.634 1.00 17.78 B ATOM 2908 OGI THR 256 17.950 55.557 35.250 1.00 10.778 B ATOM 2909 N CG THR 256 17.950 55.5654 37.105 1.00 10.778 B ATOM 2909 N CG THR 256 17.950 55.5654 37.506 1.00 17.78 B ATOM 2901 CG2 THR 256 17.950 56.564 37.521 1.00 10.75 B ATOM 2901 CG2 THR 256 17.950 56.564 37.506 1.00 23.15 B ATOM 2901 CG2 THR 256 17.950 56.564 37.523 1.00 10.778 B ATOM 2901 CG2 THR 256 19.507 58.326 37.105 1.00 10.75 B ATOM 2911 C THR 256 19.507 58.326 37.506 1.00 17.78 B ATOM 2911 C THR 256 19.507 58.326 37.506 1.00 17.78 B ATOM 2911 C THR 256 19.507 58.326 37.506 1.00 10.75 B ATOM 2913 N ASP 257 17.739 54.948 37.581 1.00 15.42 B ATOM 2913 N ASP 257 17.739 54.948 37.581 1.00 15.42 B ATOM 2913 N ASP 257 17.739 54.948 37.581 1.00 15.42 B ATOM 2913 N ASP 257 17.739 54.948 37.581 1.00 15.42 B ATOM 2913 O ASP 257 17.739 54.948 37.581 1.00 15.42 B ATOM 2913 O ASP 257 17.739 54.948 37.581 1.00 15.42 B ATOM 2913 O ASP 257 17.739 54.948 37.581 1.00 15.42 B ATOM 2913 O ASP 257 17.739 54.948 37.581 1.00 15.42 B ATOM 2913 O ASP 257 15.492 53.197 39.107 1.00 16.65 B ATOM 2913 O ASP 257 15.492 53.197 39.107 1.00 16.65 B ATOM 2922 N GLY 258 18.807 50.992 34.737 1.00 15.12 B ATOM 2922 N	35	ATOM	2890	CB ILE	254	19.903				
ATOM 2894 C ILE 254 11.107 62.500 30.176 1.00 26.33 B ATOM 2894 C ILE 254 19.911 61.596 34.635 1.00 21.12 B ATOM 2895 O ILE 254 21.031 61.215 34.976 1.00 18.90 B ATOM 2896 N VAL 255 18.804 61.377 35.348 1.00 16.92 B ATOM 2897 H VAL 255 18.796 60.692 36.629 1.00 16.15 B ATOM 2899 CB VAL 255 18.796 60.692 36.629 1.00 16.15 B ATOM 2899 CB VAL 255 18.178 61.580 37.725 1.00 18.84 B ATOM 2900 CG1 VAL 255 18.215 60.856 39.071 1.00 10.30 B ATOM 2901 CG2 VAL 255 18.931 62.925 37.796 1.00 16.06 B ATOM 2902 C VAL 255 18.931 62.925 37.796 1.00 16.06 B ATOM 2903 O VAL 255 16.799 59.434 36.484 1.00 16.06 B ATOM 2904 N THR 256 18.584 58.301 36.781 1.00 14.62 B ATOM 2905 H THR 256 19.507 58.326 37.105 1.00 015.00 B ATOM 2907 CB THR 256 17.965 57.022 36.634 1.00 15.00 B ATOM 2909 HG1 THR 256 17.950 56.564 35.161 1.00 17.78 B ATOM 2909 HG1 THR 256 17.950 56.564 35.161 1.00 17.78 B ATOM 2909 HG1 THR 256 17.950 56.564 35.161 1.00 17.78 B ATOM 2909 HG1 THR 256 17.965 57.527 35.259 1.00 0.00 B ATOM 2909 HG1 THR 256 16.277 55.527 35.259 1.00 0.00 B ATOM 2911 C THR 256 18.542 55.557 35.259 1.00 16.43 B ATOM 2912 C THR 256 19.414 56.327 34.704 1.00 16.43 B ATOM 2912 C THR 256 19.414 56.327 34.704 1.00 16.43 B ATOM 2912 C THR 256 19.414 56.327 34.704 1.00 16.43 B ATOM 2912 C THR 256 19.414 56.327 34.704 1.00 16.43 B ATOM 2912 C ASP 257 17.739 54.948 37.881 1.00 15.12 B ATOM 2913 N ASP 257 17.739 54.948 37.881 1.00 16.43 B ATOM 2914 C B ASP 257 17.739 54.948 37.881 1.00 16.43 B ATOM 2915 CA ASP 257 16.815 54.937 37.553 1.00 16.51 B ATOM 2916 CB ASP 257 15.492 53.197 39.107 1.00 16.65 B ATOM 2917 C B ASP 257 15.492 53.197 39.107 1.00 16.65 B ATOM 2918 OD1 ASP 257 15.492 53.197 39.107 1.00 16.65 B ATOM 2918 OD1 ASP 257 15.492 53.197 39.107 1.00 16.65 B ATOM 2921 O ASP 257 15.492 53.197 39.107 1.00 16.65 B ATOM 2921 O ASP 257 15.492 53.197 39.107 1.00 16.65 B ATOM 2922 N GLY 258 18.108 51.013 36.240 1.00 17.36 B ATOM 2922 N GLY 258 18.806 50.23 44.737 1.00 15.12 B ATOM 2922 N GLY 258 18.806 50.23 44.737 1.00 10.736 B ATOM 2922 N GLY 258 18.		MOTA	2891	CG2 ILE	254	18.849				
ATOM 2894 C ILE 254 19.911 61.596 34.635 1.00 21.12 B ATOM 2895 O ILE 254 21.031 61.215 34.976 1.00 18.90 B ATOM 2896 N VAL 255 18.804 61.377 35.348 1.00 16.92 B ATOM 2898 CA VAL 255 18.796 60.692 36.629 1.00 0.00 B ATOM 2899 CB VAL 255 18.796 60.692 36.629 1.00 16.15 B ATOM 2899 CB VAL 255 18.178 61.580 37.725 1.00 18.84 B ATOM 2900 CG1 VAL 255 18.215 60.856 39.071 1.00 10.30 B ATOM 2901 CG2 VAL 255 18.931 62.925 37.796 1.00 16.06 B ATOM 2902 C VAL 255 16.799 59.484 36.484 1.00 13.71 B ATOM 2903 O VAL 255 16.799 59.480 36.109 1.00 16.40 B ATOM 2904 N THR 256 18.584 58.301 36.781 1.00 14.62 B ATOM 2905 H THR 256 17.950 56.564 35.161 1.00 17.78 B ATOM 2907 CB THR 256 17.950 55.527 35.259 1.00 0.00 B ATOM 2909 HG1 THR 256 16.277 55.527 35.259 1.00 0.00 B ATOM 2901 C THR 256 19.414 56.327 34.704 1.00 10.75 B ATOM 2911 C THR 256 19.414 56.327 34.704 1.00 10.75 B ATOM 2912 O THR 256 19.414 56.327 34.704 1.00 10.75 B ATOM 2913 N ASP 257 17.739 54.948 37.851 1.00 16.43 B ATOM 2913 N ASP 257 17.739 54.948 37.851 1.00 16.43 B ATOM 2913 N ASP 257 17.739 54.948 37.851 1.00 16.43 B ATOM 2916 CB ASP 257 17.739 54.948 37.851 1.00 16.63 B ATOM 2917 CG ASP 257 15.782 53.2706 41.219 1.00 16.63 B ATOM 2918 ODI ASP 257 15.782 53.2706 41.219 1.00 16.63 B ATOM 2919 ODZ ASP 257 15.782 53.2706 41.219 1.00 16.63 B ATOM 2919 ODZ ASP 257 15.492 53.271 39.107 1.00 16.63 B ATOM 2919 ODZ ASP 257 15.782 53.2706 41.219 1.00 16.65 B ATOM 2920 C ASP 257 15.492 53.273 36.389 1.00 17.76 B ATOM 2919 ODZ ASP 257 15.782 53.2706 41.219 1.00 16.65 B ATOM 2920 C ASP 257 15.782 53.2706 41.219 1.00 16.65 B ATOM 2921 C ASP 257 15.782 53.2706 41.219 1.00 16.63 B ATOM 2922 N GLY 258 18.108 51.013 36.240 1.00 17.36 B ATOM 2924 CA GLY 258 18.108 51.013 36.240 1.00 17.36 B ATOM 2925 C GLY 258 18.328 49.792 34.159 1.00 16.87 B		ATOM	2892	CG1 ILE	254					
ATOM		MOTA	2893	CD1 ILE	254					
ATOM 2896 N VAL 255 18.804 61.377 35.348 1.00 16.92 B ATOM 2897 H VAL 255 17.951 61.700 34.986 1.00 0.00 B ATOM 2899 CB VAL 255 18.796 60.692 36.629 1.00 16.15 B ATOM 2899 CB VAL 255 18.178 61.580 37.725 1.00 18.84 B ATOM 2900 CGI VAL 255 18.215 60.856 39.071 1.00 10.30 B ATOM 2901 CG2 VAL 255 18.931 62.925 37.96 1.00 16.06 B ATOM 2902 C VAL 255 17.970 59.434 36.484 1.00 13.71 B ATOM 2903 O VAL 255 16.799 59.480 36.109 1.00 16.40 B ATOM 2904 N THR 256 18.584 58.301 36.484 1.00 14.62 B ATOM 2905 H THR 256 19.507 58.326 37.105 1.00 0.00 B ATOM 2906 CA THR 256 17.906 57.022 36.634 1.00 15.00 B ATOM 2909 NGI THR 256 17.950 56.564 35.161 1.00 17.78 B ATOM 2909 HGI THR 256 17.950 56.564 35.161 1.00 17.78 B ATOM 2909 HGI THR 256 16.277 55.527 35.259 1.00 0.00 B ATOM 2910 CG2 THR 256 19.414 56.327 34.704 1.00 10.75 B ATOM 2911 C THR 256 18.542 55.954 37.523 1.00 16.43 B ATOM 2912 O THR 256 18.542 55.954 37.523 1.00 16.31 B ATOM 2914 H ASP 257 17.739 54.948 37.881 1.00 15.42 B ATOM 2915 CA ASP 257 17.739 54.948 37.881 1.00 15.42 B ATOM 2916 CB ASP 257 16.815 54.937 37.553 1.00 16.63 B ATOM 2916 CB ASP 257 17.481 53.872 38.745 1.00 15.12 B ATOM 2918 ODI ASP 257 15.492 53.273 39.107 1.00 10.75 B ATOM 2918 ODI ASP 257 15.492 53.273 39.107 1.00 10.75 B ATOM 2918 ODI ASP 257 15.492 53.273 39.107 1.00 15.12 B ATOM 2918 ODI ASP 257 15.492 53.273 39.107 1.00 16.63 B ATOM 2921 N ASP 257 15.492 53.273 39.107 1.00 16.63 B ATOM 2921 N ASP 257 15.492 53.273 39.107 1.00 16.63 B ATOM 2922 N GLY 258 18.177 52.337 36.839 1.00 16.51 B ATOM 2921 N ASP 257 15.492 53.197 39.107 1.00 16.65 B ATOM 2922 N GLY 258 18.177 52.337 36.839 1.00 17.76 B ATOM 2922 N GLY 258 18.177 52.337 36.839 1.00 17.36 B ATOM 2924 CA GLY 258 18.108 51.013 36.240 1.00 17.36 B ATOM 2925 C GLY 258 18.108 51.013 36.240 1.00 17.36 B ATOM 2926 O G LY 258 18.302 53.127 36.277 1.00 0.00 B ATOM 2927 N GLU 258 18.302 53.127 36.277 1.00 13.51 B ATOM 2926 O GLY 258 18.302 53.127 36.277 1.00 13.51 B		MOTA	2894	C ILE	254					
ATOM 2897 H VAL 255 17.951 61.700 34.986 1.00 0.00 B ATOM 2898 CA VAL 255 18.796 60.692 36.629 1.00 16.15 B ATOM 2899 CB VAL 255 18.178 61.580 37.725 1.00 18.84 B ATOM 2900 CG1 VAL 255 18.215 60.856 39.071 1.00 10.30 B ATOM 2901 CG2 VAL 255 18.931 62.925 37.796 1.00 16.06 B ATOM 2902 C VAL 255 16.799 59.480 36.109 1.00 16.06 B ATOM 2903 O VAL 255 16.799 59.480 36.109 1.00 16.40 B ATOM 2904 N THR 256 18.584 58.301 36.781 1.00 14.62 B ATOM 2905 H THR 256 19.507 58.326 37.105 1.00 0.00 B ATOM 2906 CA THR 256 17.906 57.022 36.634 1.00 15.00 B ATOM 2907 CB THR 256 17.906 57.022 36.634 1.00 15.00 B ATOM 2909 HG1 THR 256 17.950 56.564 35.161 1.00 17.78 B ATOM 2909 HG1 THR 256 19.414 56.327 34.704 1.00 10.75 B ATOM 2910 CG2 THR 256 19.414 56.327 34.704 1.00 10.75 B ATOM 2911 C THR 256 19.414 56.327 34.704 1.00 10.75 B ATOM 2913 N ASP 257 17.739 54.948 37.821 1.00 16.43 B ATOM 2913 N ASP 257 17.739 54.948 37.821 1.00 16.43 B ATOM 2913 N ASP 257 17.739 54.948 37.821 1.00 16.43 B ATOM 2913 N ASP 257 17.739 54.948 37.821 1.00 16.43 B ATOM 2913 N ASP 257 17.739 54.948 37.881 1.00 15.42 B ATOM 2915 CA ASP 257 16.815 54.937 37.553 1.00 0.00 B ATOM 2917 CG ASP 257 16.815 54.937 37.553 1.00 16.43 B ATOM 2918 OD1 ASP 257 17.739 54.948 37.881 1.00 15.42 B ATOM 2918 OD1 ASP 257 15.492 53.197 40.119 1.00 17.76 B ATOM 2918 OD1 ASP 257 17.481 53.974 40.119 1.00 17.76 B ATOM 2918 OD1 ASP 257 15.492 53.197 39.107 1.00 18.63 B ATOM 2921 O ASP 257 15.492 53.197 39.107 1.00 18.63 B ATOM 2921 O ASP 257 15.492 53.197 39.107 1.00 18.63 B ATOM 2922 N GLY 258 18.107 52.345 38.158 1.00 15.10 B ATOM 2922 N GLY 258 18.107 52.345 38.158 1.00 17.29 B ATOM 2922 N GLY 258 18.108 51.013 36.240 1.00 17.36 B ATOM 2922 N GLY 258 18.108 51.013 36.240 1.00 17.36 B ATOM 2922 N GLY 258 18.108 51.013 36.240 1.00 17.36 B ATOM 2922 N GLY 258 18.108 51.013 36.240 1.00 17.36 B ATOM 2922 N GLY 258 18.108 51.013 36.240 1.00 17.36 B ATOM 2922 N GLY 258 18.108 51.013 36.240 1.00 17.36 B ATOM 2922 N GLY 258 18.108 51.013 36.240 1.00 17.36 B ATOM 2922 N GLY 258 18.355	40	MOTA	2895	O ILE	254					
ATOM 2898 CA VAL 255 18.796 60.692 36.629 1.00 16.15 B ATOM 2899 CB VAL 255 18.178 61.580 37.7725 1.00 18.84 B ATOM 2900 CG1 VAL 255 18.215 60.856 39.071 1.00 10.30 B ATOM 2901 CG2 VAL 255 18.931 62.925 37.796 1.00 16.06 B ATOM 2902 C VAL 255 16.799 59.484 36.484 1.00 13.71 B ATOM 2904 N THR 256 16.799 59.480 36.109 1.00 16.40 B ATOM 2905 H THR 256 19.507 58.326 37.105 1.00 0.00 B ATOM 2906 CA THR 256 17.950 56.564 35.161 1.00 17.78 B ATOM 2907 CB THR 256 17.950 56.564 35.161 1.00 17.78 B ATOM 2909 HG1 THR 256 17.950 56.564 35.161 1.00 17.78 B ATOM 2909 HG1 THR 256 16.277 55.527 35.259 1.00 0.00 B ATOM 2910 CG2 THR 256 19.414 56.327 34.704 1.00 10.75 B ATOM 2911 C THR 256 18.542 55.954 37.523 1.00 10.75 B ATOM 2912 O THR 256 19.740 56.041 37.862 1.00 16.31 B ATOM 2914 H ASP 257 16.815 54.937 37.553 1.00 16.31 B ATOM 2915 CA ASP 257 16.815 54.937 37.553 1.00 0.00 B ATOM 2916 CB ASP 257 16.815 54.937 37.553 1.00 15.42 B ATOM 2917 CG ASP 257 16.155 53.241 40.153 1.00 15.42 B ATOM 2918 OD1 ASP 257 16.155 53.241 40.153 1.00 17.76 B ATOM 2918 OD1 ASP 257 16.155 53.241 40.153 1.00 16.63 B ATOM 2919 OD2 ASP 257 15.492 53.197 40.119 1.00 17.76 B ATOM 2918 OD1 ASP 257 15.492 53.197 39.107 1.00 16.55 B ATOM 2920 C ASP 257 15.492 53.197 39.107 1.00 16.63 B ATOM 2921 O ASP 257 15.492 53.197 39.107 1.00 16.63 B ATOM 2921 O ASP 257 15.492 53.197 39.107 1.00 16.63 B ATOM 2921 O ASP 257 15.492 53.197 39.107 1.00 16.63 B ATOM 2921 O ASP 257 17.872 51.478 38.892 1.00 17.29 B ATOM 2922 N GLY 258 18.177 52.337 36.839 1.00 9.50 B ATOM 2923 H GLY 258 18.108 51.013 36.240 1.00 17.29 B ATOM 2924 CA GLY 258 18.108 51.013 36.240 1.00 17.36 B ATOM 2925 C GLY 258 18.108 51.013 36.240 1.00 17.36 B ATOM 2926 C GLY 258 18.108 50.992 34.737 1.00 13.51 B ATOM 2926 C GLY 258 18.350 52.093 34.108 1.00 17.36 B ATOM 2927 N GLU 259 18.328 49.792 34.159 1.00 16.87		MOTA	2896	N VAL	255					
ATOM 2899 CB VAL 255 18.178 61.580 37.725 1.00 18.84  45 ATOM 2901 CG1 VAL 255 18.215 60.856 39.071 1.00 10.30 B ATOM 2902 C VAL 255 18.931 62.925 37.796 1.00 16.06 B ATOM 2902 C VAL 255 17.970 59.434 36.484 1.00 13.71 B ATOM 2903 O VAL 255 16.799 59.480 36.109 1.00 16.40 B ATOM 2904 N THR 256 18.584 58.301 36.781 1.00 14.62 B ATOM 2905 H THR 256 19.507 58.326 37.105 1.00 0.00 B ATOM 2906 CA THR 256 17.906 57.022 36.634 1.00 15.00 B ATOM 2907 CB THR 256 17.950 56.564 35.161 1.00 17.78 B ATOM 2909 HG1 THR 256 16.277 55.527 35.259 1.00 0.00 B ATOM 2909 HG1 THR 256 16.277 55.527 35.259 1.00 0.00 B ATOM 2910 CG2 THR 256 19.414 56.327 34.704 1.00 10.75 B ATOM 2911 C THR 256 18.542 55.954 37.881 1.00 16.43 B ATOM 2912 O THR 256 19.740 56.041 37.862 1.00 16.43 B ATOM 2913 N ASP 257 17.739 54.948 37.881 1.00 15.42 B ATOM 2914 H ASP 257 17.739 54.948 37.881 1.00 15.42 B ATOM 2915 CA ASP 257 16.815 54.937 37.553 1.00 0.00 B ATOM 2916 CB ASP 257 17.481 53.974 40.119 1.00 15.12 B ATOM 2917 CG ASP 257 16.815 54.937 37.553 1.00 0.55 B ATOM 2918 OD1 ASP 257 15.782 52.706 41.19 1.00 15.12 B ATOM 2919 OD2 ASP 257 15.782 52.706 41.19 1.00 15.12 B ATOM 2919 OD2 ASP 257 15.782 52.706 38.158 1.00 15.10 B ATOM 2920 C ASP 257 17.872 51.478 38.992 1.00 16.55 B ATOM 2921 O ASP 257 17.872 51.478 38.992 1.00 16.55 B ATOM 2921 O ASP 257 17.872 51.478 38.992 1.00 17.29 B ATOM 2922 N GLY 258 18.302 53.127 36.277 1.00 0.00 B ATOM 2923 H GLY 258 18.302 53.127 36.277 1.00 10.00 B ATOM 2924 CA GLY 258 18.302 53.127 36.277 1.00 13.51 B ATOM 2925 C GLY 258 18.305 50.992 34.159 1.00 17.36 B ATOM 2926 O GLY 258 18.305 50.993 34.108 1.00 17.36 B ATOM 2927 N GLU 259 18.338 49.792 34.159 1.00 16.87 B		MOTA	2897	H VAL	255					
45 ATOM 2900 CG1 VAL 255 18.215 60.856 39.071 1.00 10.30 B ATOM 2901 CG2 VAL 255 18.931 62.925 37.796 1.00 16.06 B ATOM 2902 C VAL 255 17.970 59.434 36.484 1.00 13.71 B ATOM 2903 O VAL 255 16.799 59.480 36.109 1.00 16.40 B ATOM 2904 N THR 256 18.584 58.301 36.781 1.00 14.62 B ATOM 2905 H THR 256 19.507 58.326 37.105 1.00 0.00 B ATOM 2906 CA THR 256 17.906 57.022 36.634 1.00 15.00 B ATOM 2907 CB THR 256 17.950 56.544 35.161 1.00 17.78 B ATOM 2908 OG1 THR 256 17.186 55.359 35.006 1.00 23.15 B ATOM 2909 HG1 THR 256 16.277 55.527 35.259 1.00 0.00 B ATOM 2901 CG2 THR 256 19.414 56.327 34.704 1.00 10.75 B ATOM 2910 CG2 THR 256 18.542 55.954 37.821 1.00 16.31 B ATOM 2911 C THR 256 18.542 55.954 37.821 1.00 16.31 B ATOM 2913 N ASP 257 17.739 54.948 37.881 1.00 15.42 B ATOM 2914 H ASP 257 16.815 54.937 37.553 1.00 0.00 B ATOM 2915 CA ASP 257 17.481 53.974 40.119 1.00 17.76 B ATOM 2916 CB ASP 257 17.481 53.974 40.119 1.00 17.76 B ATOM 2917 CG ASP 257 15.492 53.197 39.107 1.00 16.63 B ATOM 2918 OD1 ASP 257 15.782 52.706 41.219 1.00 16.55 B ATOM 2919 OD2 ASP 257 15.492 53.197 39.107 1.00 16.63 B ATOM 2918 OD1 ASP 257 15.492 53.197 39.107 1.00 16.63 B ATOM 2920 C ASP 257 15.492 53.197 39.107 1.00 16.63 B ATOM 2921 O ASP 257 15.492 53.197 39.107 1.00 16.63 B ATOM 2921 O ASP 257 15.492 53.197 39.107 1.00 16.63 B ATOM 2921 O ASP 257 15.492 53.197 39.107 1.00 16.63 B ATOM 2921 O ASP 257 15.492 53.197 39.107 1.00 16.63 B ATOM 2921 O ASP 257 15.492 53.197 39.107 1.00 16.63 B ATOM 2922 N GLY 258 18.107 52.337 36.237 1.00 15.10 B ATOM 2923 H GLY 258 18.108 51.013 36.240 1.00 17.29 B ATOM 2924 CA GLY 258 18.302 53.127 36.277 1.00 0.00 B ATOM 2925 C GLY 258 18.302 53.127 36.277 1.00 0.00 B ATOM 2926 O GLY 258 18.350 52.038 34.108 1.00 17.36 B ATOM 2927 N GLY 258 18.350 52.038 34.108 1.00 17.36 B		MOTA	2898	CA VAL	255					
ATOM 2901 CG2 VAL 255 18.931 62.925 37.796 1.00 16.06 B ATOM 2902 C VAL 255 17.970 59.434 36.484 1.00 13.71 B ATOM 2903 O VAL 255 16.799 59.480 36.109 1.00 16.40 B ATOM 2904 N THR 256 18.584 58.301 36.781 1.00 14.62 B ATOM 2905 H THR 256 19.507 58.326 37.105 1.00 0.00 B ATOM 2906 CA THR 256 17.906 57.022 36.634 1.00 15.00 B ATOM 2907 CB THR 256 17.950 56.564 35.161 1.00 17.78 B ATOM 2908 OG1 THR 256 17.950 56.564 35.161 1.00 17.78 B ATOM 2909 HG1 THR 256 16.277 55.527 35.259 1.00 0.00 B ATOM 2909 HG1 THR 256 19.414 56.327 34.704 1.00 10.75 B ATOM 2910 CG2 THR 256 18.542 55.954 37.523 1.00 16.31 B ATOM 2911 C THR 256 18.542 55.954 37.523 1.00 16.31 B ATOM 2913 N ASP 257 17.739 54.948 37.881 1.00 15.42 B ATOM 2914 H ASP 257 16.815 54.937 37.553 1.00 0.00 B ATOM 2915 CA ASP 257 17.481 53.974 40.119 1.00 17.76 B ATOM 2916 CB ASP 257 17.481 53.974 40.119 1.00 17.76 B ATOM 2917 CG ASP 257 15.782 52.706 41.219 1.00 16.63 B ATOM 2918 OD1 ASP 257 15.782 52.706 41.219 1.00 16.63 B ATOM 2919 OD2 ASP 257 15.492 53.197 39.107 1.00 16.63 B ATOM 2919 OD2 ASP 257 15.782 52.706 41.219 1.00 16.63 B ATOM 2920 C ASP 257 15.782 52.706 41.219 1.00 16.63 B ATOM 2921 O ASP 257 15.782 52.706 41.219 1.00 16.65 B ATOM 2922 N GLY 258 18.107 52.337 36.277 1.00 0.00 B ATOM 2923 H GLY 258 18.107 52.337 36.277 1.00 0.00 B ATOM 2924 CA GLY 258 18.302 53.127 36.277 1.00 0.00 B ATOM 2925 C GLY 258 18.302 53.127 36.277 1.00 0.00 B ATOM 2926 O GLY 258 18.302 53.127 36.277 1.00 0.00 B ATOM 2926 O GLY 258 18.302 53.127 36.277 1.00 0.00 B ATOM 2926 O GLY 258 18.302 53.127 36.277 1.00 13.51 B ATOM 2926 O GLY 258 18.302 53.127 36.277 1.00 13.51 B ATOM 2926 O GLY 258 18.302 53.127 36.277 1.00 13.51 B ATOM 2926 O GLY 258 18.350 52.038 34.108 1.00 17.36 B ATOM 2927 N GLU 259 18.328 49.792 34.159 1.00 16.87		ATOM	2899	CB VAL						
ATOM 2902 C VAL 255 17.970 59.434 36.484 1.00 13.71 B ATOM 2903 O VAL 255 16.799 59.480 36.109 1.00 16.40 B ATOM 2904 N THR 256 18.584 58.301 36.781 1.00 14.62 B ATOM 2905 H THR 256 19.507 58.326 37.105 1.00 0.00 B ATOM 2906 CA THR 256 17.906 57.022 36.634 1.00 15.00 B ATOM 2907 CB THR 256 17.950 56.564 35.161 1.00 17.78 B ATOM 2908 OG1 THR 256 17.186 55.359 35.006 1.00 23.15 B ATOM 2909 HG1 THR 256 16.277 55.527 35.259 1.00 0.00 B ATOM 2910 CG2 THR 256 19.414 56.327 34.704 1.00 10.75 B ATOM 2911 C THR 256 18.542 55.954 37.523 1.00 16.31 B ATOM 2912 O THR 256 19.740 56.041 37.862 1.00 16.43 B ATOM 2913 N ASP 257 16.815 54.937 37.553 1.00 16.43 B ATOM 2914 H ASP 257 16.815 54.937 37.553 1.00 15.42 B ATOM 2916 CB ASP 257 16.815 54.937 37.553 1.00 17.76 B ATOM 2917 CG ASP 257 16.815 53.241 40.153 1.00 17.76 B ATOM 2918 OD1 ASP 257 15.782 52.706 41.219 1.00 17.76 B ATOM 2919 OD2 ASP 257 15.782 52.706 41.219 1.00 17.76 B ATOM 2918 OD1 ASP 257 15.782 52.706 41.219 1.00 17.76 B ATOM 2920 C ASP 257 15.782 52.706 41.219 1.00 17.76 B ATOM 2921 O ASP 257 15.782 52.706 41.219 1.00 17.76 B ATOM 2921 O ASP 257 15.782 52.706 41.219 1.00 16.55 B ATOM 2921 O ASP 257 15.782 52.706 41.219 1.00 16.55 B ATOM 2922 N GLY 258 18.107 52.456 38.158 1.00 15.10 B ATOM 2922 N GLY 258 18.108 51.013 36.240 1.00 17.29 B ATOM 2922 N GLY 258 18.108 51.013 36.247 1.00 15.12 B ATOM 2923 H GLY 258 18.108 51.013 36.247 1.00 15.12 B ATOM 2924 CA GLY 258 18.302 53.127 36.277 1.00 0.00 B ATOM 2924 CA GLY 258 18.302 53.127 36.277 1.00 13.51 B ATOM 2925 C GLY 258 18.328 49.992 34.159 1.00 17.36 B ATOM 2926 O GLY 258 18.328 49.992 34.737 1.00 13.51 B ATOM 2927 N GLU 259 18.328 49.992 34.159 1.00 17.36 B	45	ATOM	2900	CG1 VAL						
ATOM 2903 O VAL 255 16.799 59.480 36.109 1.00 16.40 B ATOM 2904 N THR 256 18.584 58.301 36.781 1.00 14.62 B 50 ATOM 2905 H THR 256 19.507 58.326 37.105 1.00 0.00 B ATOM 2906 CA THR 256 17.906 57.022 36.634 1.00 15.00 B ATOM 2907 CB THR 256 17.950 56.564 35.161 1.00 17.78 B ATOM 2908 OG1 THR 256 17.950 56.564 35.161 1.00 17.78 B ATOM 2909 HG1 THR 256 16.277 55.527 35.259 1.00 0.00 B 55 ATOM 2910 CG2 THR 256 19.414 56.327 34.704 1.00 10.75 B ATOM 2911 C THR 256 19.414 56.327 34.704 1.00 10.75 B ATOM 2912 O THR 256 19.740 56.041 37.862 1.00 16.31 B ATOM 2913 N ASP 257 17.739 54.948 37.881 1.00 15.42 B ATOM 2914 H ASP 257 16.815 54.937 37.553 1.00 0.00 B 60 ATOM 2915 CA ASP 257 17.481 53.974 40.119 1.00 17.76 B ATOM 2916 CB ASP 257 16.155 53.241 40.153 1.00 16.63 B ATOM 2917 CG ASP 257 15.782 52.706 41.219 1.00 16.55 B ATOM 2918 OD1 ASP 257 15.782 52.706 41.219 1.00 16.55 B ATOM 2919 OD2 ASP 257 15.782 52.706 41.219 1.00 16.55 B ATOM 2920 C ASP 257 17.872 51.478 38.892 1.00 16.55 B ATOM 2921 O ASP 257 15.782 53.197 39.107 1.00 18.63 B ATOM 2921 O ASP 257 15.782 53.197 39.107 1.00 18.63 B ATOM 2922 N GLY 258 18.107 52.337 36.839 1.00 9.50 B ATOM 2922 N GLY 258 18.108 51.013 36.240 1.00 17.29 B ATOM 2923 H GLY 258 18.302 53.127 36.277 1.00 0.00 B ATOM 2924 CA GLY 258 18.305 52.038 34.108 1.00 17.36 B ATOM 2925 C GLY 258 18.275 50.992 34.737 1.00 13.51 B ATOM 2927 N GLU 259 18.328 49.792 34.159 1.00 16.87		MOTA	2901	CG2 VAL	255					
ATOM 2904 N THR 256 18.584 58.301 36.781 1.00 14.62 B ATOM 2905 H THR 256 19.507 58.326 37.105 1.00 0.00 B ATOM 2906 CA THR 256 17.906 57.022 36.634 1.00 15.00 B ATOM 2907 CB THR 256 17.950 56.564 35.161 1.00 17.78 B ATOM 2908 OG1 THR 256 17.186 55.359 35.006 1.00 23.15 B ATOM 2909 HG1 THR 256 16.277 55.527 35.259 1.00 0.00 B  55 ATOM 2910 CG2 THR 256 19.414 56.327 34.704 1.00 10.775 B ATOM 2911 C THR 256 18.542 55.954 37.523 1.00 16.31 B ATOM 2913 N ASP 257 17.739 54.948 37.881 1.00 16.43 B ATOM 2914 H ASP 257 17.739 54.948 37.881 1.00 15.42 B ATOM 2915 CA ASP 257 16.815 54.937 37.553 1.00 0.00 B  60 ATOM 2916 CB ASP 257 17.481 53.974 40.119 1.00 17.76 B ATOM 2917 CG ASP 257 16.155 53.241 40.153 1.00 16.63 B ATOM 2918 OD1 ASP 257 15.492 53.197 39.107 1.00 16.63 B ATOM 2919 OD2 ASP 257 15.492 53.197 39.107 1.00 16.63 B ATOM 2920 C ASP 257 15.492 53.197 39.107 1.00 16.63 B ATOM 2921 O ASP 257 17.872 51.478 38.892 1.00 17.72 B ATOM 2922 N GLY 258 18.107 52.337 36.839 1.00 9.50 B ATOM 2923 H GLY 258 18.108 51.013 36.240 1.00 17.36 B ATOM 2924 CA GLY 258 18.108 51.013 36.240 1.00 17.36 B ATOM 2925 C GLY 258 18.275 50.992 34.737 1.00 13.51 B ATOM 2926 O GLY 258 18.350 52.038 34.108 1.00 17.36 B ATOM 2927 N GLU 259 18.328 49.792 34.759 1.00 13.51		ATOM	2902	C VAL	255					
50 ATOM 2905 H THR 256 19.507 58.326 37.105 1.00 0.00 B ATOM 2906 CA THR 256 17.906 57.022 36.634 1.00 15.00 B ATOM 2907 CB THR 256 17.950 56.564 35.161 1.00 17.78 B ATOM 2909 HG1 THR 256 17.186 55.359 35.006 1.00 23.15 B ATOM 2909 HG1 THR 256 16.277 55.527 35.259 1.00 0.00 B ATOM 2910 CG2 THR 256 19.414 56.327 34.704 1.00 10.75 B ATOM 2911 C THR 256 18.542 55.954 37.523 1.00 16.31 B ATOM 2912 O THR 256 19.740 56.041 37.862 1.00 16.43 B ATOM 2913 N ASP 257 17.739 54.948 37.523 1.00 16.43 B ATOM 2914 H ASP 257 16.815 54.937 37.553 1.00 0.00 B ATOM 2915 CA ASP 257 16.815 54.937 37.553 1.00 0.00 B ATOM 2916 CB ASP 257 17.481 53.974 40.119 1.00 17.76 B ATOM 2919 OD2 ASP 257 16.155 53.241 40.153 1.00 16.63 B ATOM 2919 OD2 ASP 257 15.782 52.706 41.219 1.00 16.55 B ATOM 2919 OD2 ASP 257 15.492 53.197 39.107 1.00 18.63 B ATOM 2920 C ASP 257 17.872 51.478 38.892 1.00 16.55 B ATOM 2921 O ASP 257 17.872 51.478 38.892 1.00 15.10 B ATOM 2921 O ASP 257 17.872 51.478 38.892 1.00 17.29 B ATOM 2922 N GLY 258 18.107 52.337 36.839 1.00 9.50 B ATOM 2923 H GLY 258 18.108 51.013 36.240 1.00 11.28 B ATOM 2924 CA GLY 258 18.108 51.013 36.240 1.00 11.28 B ATOM 2925 C GLY 258 18.302 53.127 36.277 1.00 0.00 B ATOM 2925 C GLY 258 18.302 53.127 36.277 1.00 13.51 B ATOM 2926 O GLY 258 18.302 53.127 36.277 1.00 13.51 B ATOM 2926 O GLY 258 18.302 52.038 34.108 1.00 17.36 B ATOM 2927 N GLU 259 18.328 49.792 34.159 1.00 16.87		MOTA	2903	O VAL						
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ATOM 2907 CB THR 256 17.950 56.564 35.161 1.00 17.78 B ATOM 2908 OG1 THR 256 17.186 55.359 35.006 1.00 23.15 B ATOM 2909 HG1 THR 256 16.277 55.527 35.259 1.00 0.00 B  55 ATOM 2910 CG2 THR 256 19.414 56.327 34.704 1.00 10.75 B ATOM 2911 C THR 256 18.542 55.954 37.523 1.00 16.31 B ATOM 2912 O THR 256 19.740 56.041 37.862 1.00 16.43 B ATOM 2913 N ASP 257 17.739 54.948 37.881 1.00 15.42 B ATOM 2914 H ASP 257 16.815 54.937 37.553 1.00 0.00 B  60 ATOM 2915 CA ASP 257 16.815 54.937 37.553 1.00 0.00 B ATOM 2916 CB ASP 257 17.481 53.974 40.119 1.00 17.76 B ATOM 2917 CG ASP 257 16.155 53.241 40.153 1.00 16.63 B ATOM 2919 OD2 ASP 257 15.782 52.706 41.219 1.00 16.55 B ATOM 2919 OD2 ASP 257 15.492 53.197 39.107 1.00 18.63 B ATOM 2920 C ASP 257 18.067 52.456 38.158 1.00 15.10 B ATOM 2921 O ASP 257 17.872 51.478 38.892 1.00 17.29 B ATOM 2922 N GLY 258 18.177 52.337 36.839 1.00 9.50 B ATOM 2923 H GLY 258 18.302 53.127 36.277 1.00 0.00 B ATOM 2924 CA GLY 258 18.302 53.127 36.277 1.00 13.51 B ATOM 2926 O GLY 258 18.305 52.038 34.108 1.00 17.36 B ATOM 2927 N GLU 259 18.328 49.792 34.159 1.00 16.87 B	50			H THR						
ATOM 2908 OG1 THR 256 17.186 55.359 35.006 1.00 23.15 B ATOM 2909 HG1 THR 256 16.277 55.527 35.259 1.00 0.00 B  55 ATOM 2910 CG2 THR 256 19.414 56.327 34.704 1.00 10.75 B ATOM 2911 C THR 256 18.542 55.954 37.523 1.00 16.31 B ATOM 2912 O THR 256 19.740 56.041 37.862 1.00 16.43 B ATOM 2913 N ASP 257 17.739 54.948 37.881 1.00 15.42 B ATOM 2914 H ASP 257 16.815 54.937 37.553 1.00 0.00 B  60 ATOM 2915 CA ASP 257 18.198 53.872 38.745 1.00 15.12 B ATOM 2916 CB ASP 257 17.481 53.974 40.119 1.00 17.76 B ATOM 2917 CG ASP 257 16.155 53.241 40.153 1.00 16.63 B ATOM 2918 OD1 ASP 257 15.782 52.706 41.219 1.00 16.55 B ATOM 2919 OD2 ASP 257 15.492 53.197 39.107 1.00 18.63 B ATOM 2920 C ASP 257 15.492 53.197 39.107 1.00 18.63 B ATOM 2921 O ASP 257 17.872 51.478 38.892 1.00 17.29 B ATOM 2922 N GLY 258 18.177 52.337 36.839 1.00 9.50 B ATOM 2923 H GLY 258 18.108 51.013 36.240 1.00 11.28 B ATOM 2924 CA GLY 258 18.108 51.013 36.240 1.00 11.28 B ATOM 2925 C GLY 258 18.275 50.992 34.737 1.00 13.51 B ATOM 2926 O GLY 258 18.328 49.792 34.159 1.00 16.87 B		MOTA	2906	CA THR						
ATOM 2909 HG1 THR 256 16.277 55.527 35.259 1.00 0.00 B ATOM 2910 CG2 THR 256 19.414 56.327 34.704 1.00 10.75 B ATOM 2911 C THR 256 18.542 55.954 37.523 1.00 16.31 B ATOM 2912 O THR 256 19.740 56.041 37.862 1.00 16.43 B ATOM 2913 N ASP 257 17.739 54.948 37.881 1.00 15.42 B ATOM 2914 H ASP 257 16.815 54.937 37.553 1.00 0.00 B ATOM 2915 CA ASP 257 18.198 53.872 38.745 1.00 15.12 B ATOM 2916 CB ASP 257 18.198 53.872 38.745 1.00 17.76 B ATOM 2916 CB ASP 257 16.155 53.241 40.153 1.00 16.63 B ATOM 2918 OD1 ASP 257 15.782 52.706 41.219 1.00 16.63 B ATOM 2919 OD2 ASP 257 15.492 53.197 39.107 1.00 18.63 B ATOM 2920 C ASP 257 15.492 53.197 39.107 1.00 18.63 B ATOM 2921 O ASP 257 17.872 52.376 38.158 1.00 15.10 B ATOM 2922 N GLY 258 18.177 52.337 36.839 1.00 9.50 B ATOM 2923 H GLY 258 18.177 52.337 36.839 1.00 9.50 B ATOM 2924 CA GLY 258 18.108 51.013 36.240 1.00 11.28 B ATOM 2925 C GLY 258 18.275 50.992 34.737 1.00 13.51 B ATOM 2926 O GLY 258 18.350 52.038 34.108 1.00 17.36 B ATOM 2927 N GLU 259 18.328 49.792 34.159 1.00 16.87 B		MOTA	2907	CB THR						
55 ATOM 2910 CG2 THR 256 19.414 56.327 34.704 1.00 10.75 B ATOM 2911 C THR 256 18.542 55.954 37.523 1.00 16.31 B ATOM 2912 O THR 256 19.740 56.041 37.862 1.00 16.43 B ATOM 2913 N ASP 257 17.739 54.948 37.881 1.00 15.42 B ATOM 2914 H ASP 257 16.815 54.937 37.553 1.00 0.00 B ATOM 2915 CA ASP 257 18.198 53.872 38.745 1.00 15.12 B ATOM 2916 CB ASP 257 17.481 53.974 40.119 1.00 17.76 B ATOM 2917 CG ASP 257 16.155 53.241 40.153 1.00 16.63 B ATOM 2918 OD1 ASP 257 15.782 52.706 41.219 1.00 16.55 B ATOM 2919 OD2 ASP 257 15.492 53.197 39.107 1.00 18.63 B ATOM 2920 C ASP 257 18.067 52.456 38.158 1.00 15.10 B ATOM 2921 O ASP 257 17.872 51.478 38.892 1.00 17.29 B ATOM 2922 N GLY 258 18.177 52.337 36.839 1.00 9.50 B ATOM 2923 H GLY 258 18.302 53.127 36.277 1.00 0.00 B ATOM 2924 CA GLY 258 18.302 53.127 36.277 1.00 0.00 B ATOM 2925 C GLY 258 18.108 51.013 36.240 1.00 11.28 B ATOM 2926 O GLY 258 18.350 52.038 34.108 1.00 17.36 B ATOM 2927 N GLU 259 18.328 49.792 34.159 1.00 16.87 B		MOTA	2908	OG1 THR	256					
ATOM 2911 C THR 256 18.542 55.954 37.523 1.00 16.31 B ATOM 2912 O THR 256 19.740 56.041 37.862 1.00 16.43 B ATOM 2913 N ASP 257 17.739 54.948 37.881 1.00 15.42 B ATOM 2914 H ASP 257 16.815 54.937 37.553 1.00 0.00 B ATOM 2916 CB ASP 257 17.481 53.974 40.119 1.00 17.76 B ATOM 2917 CG ASP 257 16.155 53.241 40.153 1.00 16.63 B ATOM 2918 OD1 ASP 257 15.782 52.706 41.219 1.00 16.55 B ATOM 2919 OD2 ASP 257 15.782 52.706 41.219 1.00 16.55 B ATOM 2920 C ASP 257 18.067 52.456 38.158 1.00 15.10 B ATOM 2921 O ASP 257 17.872 51.478 38.892 1.00 17.29 B ATOM 2922 N GLY 258 18.177 52.337 36.839 1.00 9.50 B ATOM 2923 H GLY 258 18.302 53.127 36.277 1.00 0.00 B ATOM 2924 CA GLY 258 18.302 53.127 36.277 1.00 0.00 B ATOM 2925 C GLY 258 18.108 51.013 36.240 1.00 17.36 B ATOM 2926 O GLY 258 18.275 50.992 34.737 1.00 13.51 B ATOM 2926 O GLY 258 18.350 52.038 34.108 1.00 17.36 B ATOM 2927 N GLU 259 18.328 49.792 34.159 1.00 16.87 B ATOM 2927 N GLU 259 18.328 49.792 34.159 1.00 16.87 B ATOM 2927 N GLU 259 18.328 49.792 34.159 1.00 16.87 B ATOM 2927 N GLU 259 18.328 49.792 34.159 1.00 16.87 B ATOM 2927 N GLU 259 18.328 49.792 34.159 1.00 16.87 B ATOM 2927 N GLU 259 18.328 49.792 34.159 1.00 16.87		MOTA	2909	HG1 THR						
ATOM 2911 C THR 256 18.542 55.954 37.523 1.00 16.31 B ATOM 2912 O THR 256 19.740 56.041 37.862 1.00 16.43 B ATOM 2913 N ASP 257 17.739 54.948 37.881 1.00 15.42 B ATOM 2914 H ASP 257 16.815 54.937 37.553 1.00 0.00 B ATOM 2916 CB ASP 257 18.198 53.872 38.745 1.00 15.12 B ATOM 2916 CB ASP 257 17.481 53.974 40.119 1.00 17.76 B ATOM 2917 CG ASP 257 16.155 53.241 40.153 1.00 16.63 B ATOM 2918 OD1 ASP 257 15.782 52.706 41.219 1.00 16.55 B ATOM 2919 OD2 ASP 257 15.492 53.197 39.107 1.00 18.63 B ATOM 2920 C ASP 257 18.067 52.456 38.158 1.00 15.10 B ATOM 2921 O ASP 257 17.872 51.478 38.892 1.00 17.29 B ATOM 2922 N GLY 258 18.177 52.337 36.839 1.00 9.50 B ATOM 2923 H GLY 258 18.302 53.127 36.277 1.00 0.00 B ATOM 2924 CA GLY 258 18.302 53.127 36.277 1.00 0.00 B ATOM 2925 C GLY 258 18.108 51.013 36.240 1.00 11.28 B ATOM 2926 O GLY 258 18.305 52.038 34.108 1.00 17.36 B ATOM 2927 N GLU 259 18.328 49.792 34.159 1.00 16.87 B ATOM 2927 N GLU 259 18.328 49.792 34.159 1.00 16.87 B ATOM 2927 N GLU 259 18.328 49.792 34.159 1.00 16.87 B ATOM 2927 N GLU 259 18.328 49.792 34.159 1.00 16.87 B ATOM 2927 N GLU 259 18.328 49.792 34.159 1.00 16.87 B ATOM 2927 N GLU 259 18.328 49.792 34.159 1.00 16.87 B ATOM 2927 N GLU 259 18.328 49.792 34.159 1.00 16.87 B ATOM 2927 N GLU 259 18.328 49.792 34.159 1.00 16.87	55	MOTA	2910	CG2 THR	256	19.414				
ATOM 2913 N ASP 257 17.739 54.948 37.881 1.00 15.42 B ATOM 2914 H ASP 257 16.815 54.937 37.553 1.00 0.00 B ATOM 2915 CA ASP 257 18.198 53.872 38.745 1.00 15.12 B ATOM 2916 CB ASP 257 17.481 53.974 40.119 1.00 17.76 B ATOM 2917 CG ASP 257 16.155 53.241 40.153 1.00 16.63 B ATOM 2918 OD1 ASP 257 15.782 52.706 41.219 1.00 16.55 B ATOM 2919 OD2 ASP 257 15.492 53.197 39.107 1.00 18.63 B ATOM 2920 C ASP 257 15.492 53.197 39.107 1.00 18.63 B ATOM 2921 O ASP 257 17.872 51.478 38.892 1.00 17.29 B ATOM 2922 N GLY 258 18.177 52.337 36.839 1.00 9.50 B ATOM 2923 H GLY 258 18.177 52.337 36.839 1.00 9.50 B ATOM 2924 CA GLY 258 18.302 53.127 36.277 1.00 0.00 B ATOM 2925 C GLY 258 18.108 51.013 36.240 1.00 11.28 B ATOM 2926 O GLY 258 18.305 52.038 34.108 1.00 17.36 B ATOM 2927 N GLU 259 18.328 49.792 34.737 1.00 16.87 B ATOM 2927 N GLU 259 18.328 49.792 34.159 1.00 16.87 B		MOTA	2911	C THR	256					
ATOM 2914 H ASP 257 16.815 54.937 37.553 1.00 0.00 B ATOM 2915 CA ASP 257 18.198 53.872 38.745 1.00 15.12 B ATOM 2916 CB ASP 257 17.481 53.974 40.119 1.00 17.76 B ATOM 2917 CG ASP 257 16.155 53.241 40.153 1.00 16.63 B ATOM 2918 OD1 ASP 257 15.782 52.706 41.219 1.00 16.55 B ATOM 2919 OD2 ASP 257 15.492 53.197 39.107 1.00 18.63 B ATOM 2920 C ASP 257 18.067 52.456 38.158 1.00 15.10 B ATOM 2921 O ASP 257 17.872 51.478 38.892 1.00 17.29 B ATOM 2922 N GLY 258 18.177 52.337 36.839 1.00 9.50 B ATOM 2923 H GLY 258 18.302 53.127 36.277 1.00 0.00 B ATOM 2924 CA GLY 258 18.302 53.127 36.277 1.00 0.00 B ATOM 2925 C GLY 258 18.108 51.013 36.240 1.00 11.28 B ATOM 2926 O GLY 258 18.350 52.038 34.108 1.00 17.36 B ATOM 2927 N GLU 259 18.328 49.792 34.159 1.00 16.87 B		MOTA	2912	O THR	256					
60 ATOM 2915 CA ASP 257 18.198 53.872 38.745 1.00 15.12 B ATOM 2916 CB ASP 257 17.481 53.974 40.119 1.00 17.76 B ATOM 2917 CG ASP 257 16.155 53.241 40.153 1.00 16.63 B ATOM 2918 OD1 ASP 257 15.782 52.706 41.219 1.00 16.55 B ATOM 2919 OD2 ASP 257 15.492 53.197 39.107 1.00 18.63 B ATOM 2920 C ASP 257 18.067 52.456 38.158 1.00 15.10 B ATOM 2921 O ASP 257 17.872 51.478 38.892 1.00 17.29 B ATOM 2922 N GLY 258 18.177 52.337 36.839 1.00 9.50 B ATOM 2923 H GLY 258 18.302 53.127 36.277 1.00 0.00 B ATOM 2924 CA GLY 258 18.302 53.127 36.277 1.00 0.00 B ATOM 2924 CA GLY 258 18.108 51.013 36.240 1.00 11.28 B ATOM 2925 C GLY 258 18.275 50.992 34.737 1.00 13.51 B ATOM 2926 O GLY 258 18.350 52.038 34.108 1.00 17.36 B ATOM 2927 N GLU 259 18.328 49.792 34.159 1.00 16.87 B		ATOM	2913	n Asf	257					
ATOM 2916 CB ASP 257 17.481 53.974 40.119 1.00 17.76 B ATOM 2917 CG ASP 257 16.155 53.241 40.153 1.00 16.63 B ATOM 2918 OD1 ASP 257 15.782 52.706 41.219 1.00 16.55 B ATOM 2919 OD2 ASP 257 15.492 53.197 39.107 1.00 18.63 B ATOM 2920 C ASP 257 18.067 52.456 38.158 1.00 15.10 B ATOM 2921 O ASP 257 17.872 51.478 38.892 1.00 17.29 B ATOM 2922 N GLY 258 18.177 52.337 36.839 1.00 9.50 B ATOM 2923 H GLY 258 18.302 53.127 36.277 1.00 0.00 B ATOM 2924 CA GLY 258 18.108 51.013 36.240 1.00 11.28 B ATOM 2925 C GLY 258 18.275 50.992 34.737 1.00 13.51 B ATOM 2926 O GLY 258 18.350 52.038 34.108 1.00 17.36 B ATOM 2927 N GLU 259 18.328 49.792 34.159 1.00 16.87 B		ATOM	2914	H ASF	257	16.815				
ATOM 2916 CB ASP 257 17.481 53.974 40.119 1.00 17.76 B ATOM 2917 CG ASP 257 16.155 53.241 40.153 1.00 16.63 B ATOM 2918 OD1 ASP 257 15.782 52.706 41.219 1.00 16.55 B ATOM 2919 OD2 ASP 257 15.492 53.197 39.107 1.00 18.63 B ATOM 2920 C ASP 257 18.067 52.456 38.158 1.00 15.10 B ATOM 2921 O ASP 257 17.872 51.478 38.892 1.00 17.29 B ATOM 2922 N GLY 258 18.177 52.337 36.839 1.00 9.50 B ATOM 2923 H GLY 258 18.302 53.127 36.277 1.00 0.00 B ATOM 2924 CA GLY 258 18.108 51.013 36.240 1.00 11.28 B ATOM 2925 C GLY 258 18.275 50.992 34.737 1.00 13.51 B ATOM 2926 O GLY 258 18.350 52.038 34.108 1.00 17.36 B ATOM 2927 N GLU 259 18.328 49.792 34.159 1.00 16.87 B	60	ATOM	2915	CA ASF	257	18.198				
ATOM 2917 CG ASP 257 16.155 53.241 40.153 1.00 16.63 B ATOM 2918 OD1 ASP 257 15.782 52.706 41.219 1.00 16.55 B ATOM 2919 OD2 ASP 257 15.492 53.197 39.107 1.00 18.63 B ATOM 2920 C ASP 257 18.067 52.456 38.158 1.00 15.10 B ATOM 2921 O ASP 257 17.872 51.478 38.892 1.00 17.29 B ATOM 2922 N GLY 258 18.177 52.337 36.839 1.00 9.50 B ATOM 2923 H GLY 258 18.302 53.127 36.277 1.00 0.00 B ATOM 2924 CA GLY 258 18.108 51.013 36.240 1.00 11.28 B ATOM 2925 C GLY 258 18.275 50.992 34.737 1.00 13.51 B ATOM 2926 O GLY 258 18.350 52.038 34.108 1.00 17.36 B ATOM 2927 N GLU 259 18.328 49.792 34.159 1.00 16.87 B		ATOM	2916	CB ASF	257	17.481		40.119		
ATOM 2918 OD1 ASP 257 15.782 52.706 41.219 1.00 16.55 B ATOM 2919 OD2 ASP 257 15.492 53.197 39.107 1.00 18.63 B ATOM 2920 C ASP 257 18.067 52.456 38.158 1.00 15.10 B ATOM 2921 O ASP 257 17.872 51.478 38.892 1.00 17.29 B ATOM 2922 N GLY 258 18.177 52.337 36.839 1.00 9.50 B ATOM 2923 H GLY 258 18.302 53.127 36.277 1.00 0.00 B ATOM 2924 CA GLY 258 18.108 51.013 36.240 1.00 11.28 B ATOM 2925 C GLY 258 18.275 50.992 34.737 1.00 13.51 B ATOM 2926 O GLY 258 18.350 52.038 34.108 1.00 17.36 B ATOM 2927 N GLU 259 18.328 49.792 34.159 1.00 16.87 B			2917	CG ASF	257	16.155		40.153		
ATOM 2919 OD2 ASP 257 15.492 53.197 39.107 1.00 18.63 B ATOM 2920 C ASP 257 18.067 52.456 38.158 1.00 15.10 B ATOM 2921 O ASP 257 17.872 51.478 38.892 1.00 17.29 B ATOM 2922 N GLY 258 18.177 52.337 36.839 1.00 9.50 B ATOM 2923 H GLY 258 18.302 53.127 36.277 1.00 0.00 B ATOM 2924 CA GLY 258 18.108 51.013 36.240 1.00 11.28 B ATOM 2925 C GLY 258 18.275 50.992 34.737 1.00 13.51 B ATOM 2926 O GLY 258 18.350 52.038 34.108 1.00 17.36 B ATOM 2927 N GLU 259 18.328 49.792 34.159 1.00 16.87 B			2918	OD1 ASF	257	15.782	52.706			
ATOM 2921 O ASP 257 17.872 51.478 38.892 1.00 17.29 B ATOM 2922 N GLY 258 18.177 52.337 36.839 1.00 9.50 B ATOM 2923 H GLY 258 18.302 53.127 36.277 1.00 0.00 B ATOM 2924 CA GLY 258 18.108 51.013 36.240 1.00 11.28 B ATOM 2925 C GLY 258 18.275 50.992 34.737 1.00 13.51 B ATOM 2926 O GLY 258 18.350 52.038 34.108 1.00 17.36 B ATOM 2927 N GLU 259 18.328 49.792 34.159 1.00 16.87 B			2919	OD2 ASE	257	15.492				
ATOM 2921 O ASP 257 17.872 51.478 38.892 1.00 17.29 B ATOM 2922 N GLY 258 18.177 52.337 36.839 1.00 9.50 B ATOM 2923 H GLY 258 18.302 53.127 36.277 1.00 0.00 B ATOM 2924 CA GLY 258 18.108 51.013 36.240 1.00 11.28 B ATOM 2925 C GLY 258 18.275 50.992 34.737 1.00 13.51 B ATOM 2926 O GLY 258 18.350 52.038 34.108 1.00 17.36 B ATOM 2927 N GLU 259 18.328 49.792 34.159 1.00 16.87 B	65			C ASE	257	18.067				
ATOM 2922 N GLY 258 18.177 52.337 36.839 1.00 9.50 B ATOM 2923 H GLY 258 18.302 53.127 36.277 1.00 0.00 B ATOM 2924 CA GLY 258 18.108 51.013 36.240 1.00 11.28 B ATOM 2925 C GLY 258 18.275 50.992 34.737 1.00 13.51 B ATOM 2926 O GLY 258 18.350 52.038 34.108 1.00 17.36 B ATOM 2927 N GLU 259 18.328 49.792 34.159 1.00 16.87 B	-			O ASE	257	17.872			1.00 17.29	
ATOM 2923 H GLY 258 18.302 53.127 36.277 1.00 0.00 B ATOM 2924 CA GLY 258 18.108 51.013 36.240 1.00 11.28 B ATOM 2925 C GLY 258 18.275 50.992 34.737 1.00 13.51 B ATOM 2926 O GLY 258 18.350 52.038 34.108 1.00 17.36 B ATOM 2927 N GLU 259 18.328 49.792 34.159 1.00 16.87 B										В
ATOM 2924 CA GLY 258 18.108 51.013 36.240 1.00 11.28 B 70 ATOM 2925 C GLY 258 18.275 50.992 34.737 1.00 13.51 B ATOM 2926 O GLY 258 18.350 52.038 34.108 1.00 17.36 B ATOM 2927 N GLU 259 18.328 49.792 34.159 1.00 16.87 B						18.302		36.277		В
70 ATOM 2925 C GLY 258 18.275 50.992 34.737 1.00 13.51 B ATOM 2926 O GLY 258 18.350 52.038 34.108 1.00 17.36 B ATOM 2927 N GLU 259 18.328 49.792 34.159 1.00 16.87 B						18.108				В
ATOM 2926 O GLY 258 18.350 52.038 34.108 1.00 17.36 B ATOM 2927 N GLU 259 18.328 49.792 34.159 1.00 16.87 B	70					18.275				В
ATOM 2927 N GLU 259 18.328 49.792 34.159 1.00 16.87 B	-					18.350		34.108		В
10 0FF 40 00F 34 700 1 00 0 00										В
						18.257	48.995	34.723	1.00 0.00	В

	ATOM	2929	CA GLU	259	18.488	49.628	32.718	1.00 20.62	В
	MOTA	2930	CB GLU	259	18.730	48.158	32.358	1.00 23.36	B B
	ATOM	2931	CG GLU	259	20.115 20.119	47.652 46.175	32.667 33.015	1.00 32.72 1.00 31.78	В
5	ATOM	2932	CD GLU OE1 GLU	259 259	19.803	45.356	32.120	1.00 30.21	В
3	ATOM ATOM	2933 2934	OE1 GLU OE2 GLU	259	20.441	45.844	34.178	1.00 27.13	B
	ATOM	2935	C GLU	259	17.238	50.083	32.003	1.00 22.02	В
	ATOM	2936	O GLU	259	16.141	50.060	32.571	1.00 22.92	В
	MOTA	2937	N SER	260	17.383	50.452	30.736	1.00 17.73	В
10	MOTA	2938	H SER	260	18.264	50.419	30.314	1.00 0.00	В
	MOTA	2939	CA SER	260	16.226	50.900	29.987 29.133	1.00 21.31 1.00 18.50	B B
	MOTA	2940	CB SER	260	16.609 17.456	52.107 51.716	28.080	1.00 18.50	В
	MOTA	2941 2942	OG SER HG SER	260 260	18.255	51.324	28.441	1.00 0.00	B
15	ATOM ATOM	2943	C SER	260	15.619	49.794	29.109	1.00 16.77	В
15	MOTA	2944	O SER	260	16.330	49.027	28.486	1.00 16.79	В
	ATOM	2945	N HIS	261	14.292	49.719	29.083	1.00 20.77	В
	MOTA	2946	H HIS	261	13.775	50.351	29.622	1.00 0.00	В
20	MOTA	2947	CA HIS	261	13.581	48.730 48.819	28.280 28.545	1.00 26.28 1.00 36.28	B B
20	ATOM	2948	CB HIS	261 261	12.074 11.565	47.849	29.564	1.00 47.66	В
	ATOM ATOM	29 <b>4</b> 9 2950	CD2 HIS	261	10.832	46.717	29.426	1.00 49.49	В
	MOTA	2951	ND1 HIS	261	11.764	48.015	30.919	1.00 51.66	В
	MOTA	2952	HD1 HIS	261	12.252	48.757	31.331	1.00 0.00	В
25	MOTA	2953	CE1 HIS	261	11.170	47.034	31.575	1.00 50.93	B B
	ATOM	2954	NE2 HIS	261	10.599	46.231 45.430	30.693 30.904	1.00 52.42 1.00 0.00	В
	ATOM	2955 2956	HE2 HIS	261 261	10.085 13.836	49.169	26.854	1.00 23.53	В
	MOTA MOTA	2957	O HIS	261	13.634	48.437	25.895	1.00 23.83	В
30	ATOM	2958	N TYR	262	14.292	50.405	26.767	1.00 22.41	В
	ATOM	2959	H TYR	262	14.447	50.886	27.607	1.00 0.00	В
	MOTA	2960	CA TYR	262	14.581	51.112	25.537	1.00 22.32	B B
	ATOM	2961	CB TYR	262	14.348 13.305	52.594 53.169	25.795 24.914	1.00 29.85 1.00 35.37	В
35	ATOM ATOM	2962 2963	CG TYR	262 262	12.587	54.264	25.316	1.00 29.84	В
33	ATOM	2964	CE1 TYR	262	11.582	54.781	24.522	1.00 46.06	В
	ATOM	2965	CD2 TYR	262	13.009	52.594	23.671	1.00 41.64	В
	ATOM	2966	CE2 TYR	262	11.987	53.118	22.858	1.00 46.38	В
4.0	MOTA	2967	CZ TYR	262	11.281	54.224	23.302	1.00 41.00 1.00 44.86	В В
40	ATOM	2968	OH TYR	262 262	10.252 10.120	54.782 54.276	22.570 21.766	1.00 44.80	В
	MOTA MOTA	2969 2970	HH TYR	262	15.981	50.955	24.943	1.00 21.72	В
	ATOM	2971	O TYR	262	16.269	51.550	23.903	1.00 17.28	В
	ATOM	2972	N ASN	263	16.839	50.201	25.628	1.00 23.04	В
45	ATOM	2973	H ASN		16.526	49.784	26.457	1.00 0.00	B B
	MOTA	2974	CA ASN		18.222 18.634	49.950 48.513	25.220 25.584	1.00 24.13 1.00 29.95	В
	ATOM	2975 2976	CB ASN		18.971	48.335	27.058	1.00 36.99	В
	MOTA MOTA	2977	OD1 ASN		18.731	49.210	27.886	1.00 41.66	В
50	ATOM	2978	ND2 ASN		19.528	47.181	27.384	1.00 40.94	В
	MOTA		HD21 ASN	263	19.702	46.507	26.693	1.00 0.00	В
	MOTA		HD22 ASN		19.752	47.038	28.326 23.736	1.00 0.00 1.00 23.55	В В
	ATOM	2981	C ASN		18.543 19.316	50.136 51.006	23.736	1.00 23.33	В
55	ATOM ATOM	2982 2983	O ASN N HIS		17.958	49.279	22.900	1.00 23.91	В
55	MOTA	2984	H HIS		17.341	48.618	23.274	1.00 0.00	В
	ATOM	2985	CA HIS	264	18.189	49.276	21.458	1.00 26.11	В
	ATOM	2986	CB HIS		17.205	48.308	20.778	1.00 23.47	В
<b>60</b>	MOTA	2987	CG HIS		15.766 14.846	48.685 48.294	20.947 21.863	1.00 22.25 1.00 24.90	B B
60	MOTA	2988 2989	CD2 HIS		15.129	49.594	20.131	1.00 23.90	В
	MOTA MOTA	2990	HD1 HIS		15.530	50.056	19.366	1.00 0.00	В
	ATOM	2991	CE1 HIS		13.881	49.748	20.532	1.00 31.00	В
	ATOM	2992	NE2 HIS		13.683	48.970	21.586	1.00 28.44	В
65	ATOM	2993	HE2 HIS		12.847	48.889	22.081	1.00 0.00	В
	ATOM	2994	C HIS		18.163	50.601	20.706	1.00 29.92 1.00 31.12	B B
	ATOM	2995	O HIS		18.712 17.527	50.710 51.613	19.614 21.282	1.00 31.12	В
	MOTA MOTA	2996 2997	N ARG		17.125	51.493	22.161	1.00 0.00	В
70	ATOM	2998	CA ARG		17.435	52.905	20.619	1.00 33.48	В
, 0	ATOM	2999	CB ARG		16.140	53.580	21.011	1.00 35.96	В
	MOTA	3000	CG ARG	265	14.909		20.585	1.00 43.13	В
	MOTA	3001	CD ARG	265	14.090	53.926	19.852	1.00 45.62	В

							00 555	1 00 41 00	Ъ
	MOTA		ARG	265	13.403	54.838 54.478	20.755 21.594	1.00 41.09 1.00 0.00	B B
	ATOM		ARG ARG	265 265	13.054 13.218	56.130	20.506	1.00 42.46	В
	ATOM ATOM	3004 CZ 3005 NH1		265	13.671	56.670	19.380	1.00 43.62	В
5	MOTA	3006 HH11		265	14.151	56.104	18.710	1.00 0.00	В
•	MOTA	3007 HH12		265	13.529	57.644	19.202	1.00 0.00	В
	MOTA	3008 NH2		265	12.565	56.879	21.374	1.00 43.11 1.00 0.00	B B
	ATOM	3009 HH21		265	12.206 12.426	56.472 57.852	22.213 21.189	1.00 0.00 1.00 0.00	В
10	ATOM	3010 HH22 3011 C	ARG	265 265	18.535	53.875	21.100	1.00 31.98	B
10	MOTA MOTA		ARG	265	18.666	54.954	20.443	1.00 25.36	В
	MOTA		LEU	266	19.302	53.472	22.059	1.00 27.18	В
	ATOM		LEU	266	19.231	52.547	22.360	1.00 0.00	В
	MOTA	3015 CA	LEU	266	20.303	54.346	22.685	1.00 26.54	В
15	ATOM		LEU	266	20.987	53.646	23.864	1.00 21.25	B B
	MOTA		LEU	266	20.178	53.787	25.158 26.265	1.00 23.40 1.00 16.18	В
	ATOM	3018 CD1		266 266	20.950 19.900	53.117 55.260	25.505	1.00 13.13	В
	ATOM ATOM	3019 CD2 3020 C	LEU	266	21.337	54.990	21.809	1.00 28.09	В
20	MOTA	3021 0	LEU	266	21.467	56.208	21.838	1.00 30.85	В
20	ATOM	3022 N	GLN	267	22.045	54.199	21.031	1.00 29.76	В
	MOTA	3023 H	GLN	267	21.873	53.236	21.016	1.00 0.00	В
	MOTA	3024 CA	GLN	267	23.086	54.733	20.162	1.00 29.56 1.00 36.52	B B
25	MOTA	3025 CB	GLN	267	23.692 23.964	53.605 52.362	19.344 20.169	1.00 50.23	В
25	ATOM	3026 CG 3027 CD	GLN GLN	267 267	23.778	51.084	19.380	1.00 58.15	В
	ATOM ATOM	3027 CD 3028 OE1		267	23.350	50.056	19.919	1.00 60.56	В
	ATOM	3029 NE2		267	24.100	51.138	18.089	1.00 62.36	В
	MOTA	3030 HE21	GLN	267	24.434	51.976	17.706	1.00 0.00	В
30	MOTA	3031 HE22		267	23.988	50.324	17.561	1.00 0.00 1.00 31.18	B B
	MOTA	3032 C	GLN	267	22.556 23.145	55.825 56.905	19.245 19.130	1.00 31.18	В
	MOTA MOTA	3033 O 3034 N	GLN LYS	267 268	21.443	55.540	18.582	1.00 29.62	В
	ATOM	3035 H	LYS	268	21.009	54.672	18.704	1.00 0.00	В
35	ATOM	3036 CA	LYS	268	20.872	56.514	17.687	1.00 26.36	В
	MOTA	3037 CB	LYS	268	19.650	55.937	16.976	1.00 29.19	В В
	MOTA	3038 CG	LYS	268	19.037	56.897 57.194	15.952 14.800	1.00 37.26 1.00 37.93	В
	MOTA	3039 CD 3040 CE	LYS LYS	268 268	20.002 19.555	56.514	13.516	1.00 45.23	В
40	ATOM ATOM	3040 CE 3041 NZ	LYS	268	20.397	56.862	12.327	1.00 50.96	В
40	MOTA		LYS	268	21.379	56.574	12.501	1.00 0.00	В
	MOTA		LYS	268	20.358	57.888	12.163	1.00 0.00	В
	MOTA		LYS	268	20.032	56.365	11.488	1.00 0.00	B B
4.~	MOTA	3045 C	LYS	268	20.476 20.834	57.755 58.864	18.464 18.085	1.00 22.33 1.00 18.43	В
45	MOTA ATOM	3046 O 3047 N	LYS VAL	268 269	19.744	57.570	19.556	1.00 25.38	B
	ATOM	3047 N	VAL	269	19.505	56.659	19.828	1.00 0.00	В
	ATOM	3049 CA	VAL	269	19.294	58.706	20.357	1.00 24.60	В
	ATOM		VAL	269	18.422	58.270	21.562	1.00 21.43	В
50	ATOM		VAL	269	18.359	59.395	22.582	1.00 20.07 1.00 13.06	B B
	ATOM		VAL	269 269	17.014 20.471	57.926 59.518	21.092 20.876	1.00 15.00	В
	ATOM ATOM	3053 C 3054 O	VAL VAL	269	20.453	60.753	20.827	1.00 24.64	В
	ATOM	3055 N	ILE	270	21.494	58.830	21.372	1.00 25.28	В
55	ATOM	3056 Н	ILE	270	21.457	57.854	21.397	1.00 0.00	В
	MOTA	3057 CA	ILE	270	22.674	59.520	21.878	1.00 20.75	В
	MOTA	3058 CB	ILE	270	23.657	58.535	22.568 22.813	1.00 22.70 1.00 16.22	В В
	ATOM	3059 CG2	ILE ILE	270 270	25.019 23.078	59.210 58.064	23.912	1.00 10.22	В
60	ATOM ATOM		ILE	270	21.829	58.794	24.368	1.00 28.95	В
00	ATOM	3062 C	ILE	270	23.377	60.244	20.730	1.00 24.26	В
	ATOM	3063 0	ILE	270	23.877	61.350	20.919	1.00 25.59	В
	ATOM	3064 N	GLN	271	23.387	59.646	19.538	1.00 24.44	В
	MOTA	3065 H	GLN	271	22.937	58.783	19.424	1.00 0.00 1.00 24.78	В В
65	ATOM	3066 CA	GLN	271	24.066 24.125	60.269 59.335	18.389 17.186	1.00 24.78	В
	ATOM	3067 CB 3068 CG	GLN GLN	271 271	24.125	59.333	16.040	1.00 26.49	В
	ATOM ATOM	3068 CG 3069 CD	$_{\rm GLN}$	271	26.371	60.238	16.481	1.00 29.28	В
	ATOM		GLN	271	26.939	61.274	16.127	1.00 30.26	В
70	ATOM	3071 NE2	GLN	271	26.951	59.345	17.264	1.00 30.30	В
	MOTA	3072 HE21		271	26.460	58.535	17.522	1.00 0.00	B B
	ATOM	3073 HE22		271	27.862 23.404	59.527 61.550	17.562 17.944	1.00 0.00 1.00 24.46	B B
	MOTA	3074 C	GLN	271	40.404	01.550	11.Jus		_

	ATOM	3075	O GLN	271	24.067	62.496	17.509	1.00 16.78	В
	ATOM	3076 3077	N ASP	272 272	22.082 21.615	61.557 60.756	18.025 18.343	1.00 21.10 1.00 0.00	B B
	ATOM ATOM	3077	H ASP	272	21.325	62.718	17.650	1.00 17.66	В
5	MOTA	3079	CB ASP	272	19.848	62.340 61.417	17.563 16.376	1.00 21.71 1.00 24.50	B B
	ATOM ATOM	3080 3081	CG ASP	272 272	19.567 20.276	61.541	15.361	1.00 24.30	В
	ATOM	3082	OD2 ASP	272	18.656	60.571	16.449	1.00 28.77	В
10	ATOM	3083	C ASP O ASP	272 272	21.593 21.699	63.832 64.997	18.656 18.284	1.00 17.80 1.00 18.02	B B
10	ATOM ATOM	3084 3085	O ASP N CYS	273	21.729	63.477	19.931	1.00 18.60	В
	ATOM	3086	H CYS	273	21.636	62.537	20.187	1.00 0.00	B B
	MOTA MOTA	3087 3088	CA CYS	273 273	22.022 22.050	64.488 63.867	20.945 22.347	1.00 20.63 1.00 16.54	В
15	ATOM	3089	SG CYS	273	20.445	63.515	23.095	1.00 35.11	В
	MOTA	3090	C CYS	273	23.396 23.579	65.085 66.305	20.641 20.707	1.00 23.93 1.00 21.34	B B
	MOTA MOTA	3091 3092	O CYS	273 274	24.346	64.212	20.707	1.00 21.52	В
	MOTA	3093	H GLU	274	24.114	63.261	20.261	1.00 0.00	В
20	ATOM	3094	CA GLU	274 274	25.723 26.523	64.601 63.355	19.993 19.575	1.00 25.93 1.00 25.37	B B
	ATOM ATOM	3095 3096	CB GLU	274	28.017	63.412	19.847	1.00 33.76	В
	MOTA	3097	CD GLU	274	28.381	64.114	21.149	1.00 35.86	B B
25	ATOM ATOM	3098 3099	OE1 GLU OE2 GLU	274 274	29.384 27.682	64.855 63.929	21.154 $22.164$	1.00 39.26 1.00 31.65	В
23	ATOM	3100	C GLU	274	25.801	65.667	18.896	1.00 27.29	В
	MOTA	3101	O GLU	274	26.479 25.110	66.692 65.409	19.055 17.786	1.00 21.91 1.00 25.89	B B
	ATOM ATOM	3102 3103	N ASP H ASP	275 275	24.605	64.571	17.736	1.00 0.00	В
30	ATOM	3104	CA ASP	275	25.069	66.319	16.635	1.00 29.31	В
	MOTA MOTA	3105 3106	CB ASP	275 275	24.320 25.031	65.655 64.420	15.471 14.938	1.00 28.05 1.00 37.38	B B
	MOTA	3107	OD1 ASP	275	26.257	64.293	15.145	1.00 41.51	В
25	ATOM	3108	OD2 ASP	275	24.360 24.408	63.575 67.674	14.305 16.939	1.00 34.32 1.00 29.09	B B
35	MOTA MOTA	3109 3110	C ASP O ASP	275 275	24.408	68.679	16.268	1.00 22.13	В
	MOTA	3111	N GLU	276	23.529	67.688	17.935 18.423	1.00 30.74 1.00 0.00	B B
	ATOM ATOM	3112 3113	H GLU CA GLU	276 276	23.353 22.817	66.859 68.901	18.423	1.00 0.00	В
40	MOTA	3114	CB GLU	276	21.403	68.554	18.792	1.00 31.31	В
	ATOM	3115	CG GLU		20.404 19.015	68.622 68.175	17.654 18.049	1.00 35.70 1.00 42.31	B B
	ATOM ATOM	3116 3117	CD GLU OE1 GLU		18.415	67.389	17.284	1.00 40.50	В
4.5	MOTA	3118	OE2 GLU		18.521	68.606 69.557	19.115 19.431	1.00 46.76 1.00 29.44	B B
45	ATOM ATOM	3119 3120	C GLU		23.606 23.234	70.604	19.968	1.00 24.35	В
	ATOM	3121	n Asn	277	24.727	68.918	19.744	1.00 28.11	В
	ATOM	3122 3123	H ASN		24.942 25.644	68.087 69.401	19.272 20.757	1.00 0.00 1.00 29.61	B B
50	ATOM ATOM	3123 $3124$	CB ASN		26.309	70.682	20.271	1.00 32.09	В
	ATOM	3125	CG ASN		27.387	70.398	19.252 19.597	1.00 38.92 1.00 38.13	B B
	MOTA MOTA	3126 3127	OD1 ASN ND2 ASN		28. <b>4</b> 55 27.113	69.880 70.712	17.989	1.00 39.28	В
	MOTA	3128	HD21 ASN	277	26.245	71.104	17.760	1.00 0.00	В
55	ATOM		HD22 ASN		27.804 25.023	70.534 69.617	17.319 22.111	1.00 0.00 1.00 27.06	В В
	MOTA MOTA	3130 3131	C ASN		25.118	70.691	22.693	1.00 28.18	В
	MOTA	3132	N ILE	278	24.390	68.572	22.613	1.00 22.45 1.00 0.00	B B
60	ATOM ATOM	3133 3134	H ILE		24.339 23.775	67.740 68.640	22.096 23.909	1.00 0.00 1.00 18.31	В
00	ATOM	3135	CB ILE		22.422	67.904	23.899	1.00 14.49	В
	MOTA	3136	CG2 ILE		21.895	67.787	25.306 22.962	1.00 12.68 1.00 17.11	B B
	ATOM ATOM	3137 3138	CG1 ILE		21.454 20.093	68.639 68.024	22.870	1.00 17.11	В
65	MOTA	3139	C ILE	278	24.728	67.978	24.903	1.00 18.85	В
	ATOM	3140	O ILE N GLN		25.052 25.180	66.802 68.738	24.767 25.896	1.00 17.29 1.00 15.07	В В
	ATOM ATOM	3141 3142	N GLN H GLN		24.907	69.676	25.956	1.00 0.00	В
	MOTA	3143	CA GL1	279	26.071	68.182	26.891	1.00 20.54	В В
70	MOTA MOTA	3144 3145	CB GL1 CG GL1		26.788 28.008	69.299 68.836	27.636 28.428	1.00 22.04 1.00 25.39	В
	ATOM	3145	CD GL1	279	28.683	69.984	29.146	1.00 25.91	В
	MOTA	3147	OE1 GLM	1 279	29.500	69.777	30.040	1.00 26.55	В

	ATOM	3148	NE2	GLN	279	28.340	71.208	28.758	1.00 23.93	В
	MOTA		HE21 (		279	27.685	71.328	28.040	1.00 0.00	В
	MOTA		HE22 (		279	28.769	71.963	29.211	1.00 0.00 1.00 17.77	B B
_	ATOM	3151		GLN	279 279	25.253 24.310	67.347 67.847	27.866 28.475	1.00 17.77	В
5	ATOM ATOM	3152 3153		GLN ARG	280	25.620	66.081	28.025	1.00 19.35	В
	ATOM	3153		ARG	280	26.398	65.742	27.538	1.00 0.00	B
	ATOM	3155		ARG	280	24.880	65.184	28.913	1.00 17.76	В
	ATOM	3156		ARG	280	24.285	64.007	28.123	1.00 13.32	В
10-	ATOM	3157		ARG	280	24.065	64.255	26.641	1.00 16.90	В
	MOTA	3158	CD :	ARG	280	23.912	62.956	25.872	1.00 12.99	В
	MOTA	3159	NE .	ARG	280	25.175	62.404	25.368	1.00 14.94	В
	MOTA	3160		ARG	280	25.533	61.605	25.802	1.00 0.00	В
	ATOM	3161		ARG	280	25.866	62.931	24.363	1.00 18.57 1.00 16.91	B B
15	MOTA	3162	NH1.		280	25.421 24.569	64.025 64.453	23.754 24.058	1.00 10.91	В
	MOTA		HH11 .		280 280	25.937	64.433	22.996	1.00 0.00	В
	ATOM ATOM	3165	NH2		280	27.005	62.370	23.965	1.00 12.64	В
	ATOM		HH21		280	27.344	61.552	24.430	1.00 0.00	В
20	ATOM		HH22		280	27.521	62.763	23.211	1.00 0.00	В
20	ATOM	3168		ARG	280	25.628	64.601	30.111	1.00 16.54	В
	MOTA	3169		ARG	280	26.644	63.912	29.968	1.00 18.85	В
	ATOM	3170	N	PHE	281	25.099	64.893	31.288	1.00 14.11	В
	MOTA	3171		PHE	281	24.324	65.492	31.315	1.00 0.00	В
25	MOTA	3172		PHE	281	25.611	64.374	32.543	1.00 13.98	B B
	MOTA	3173		PHE	281	25.610	65.452 66.572	33.632 33.394	1.00 20.05 1.00 23.08	В
	ATOM	3174		PHE	281 281	26.572 26.213	67.660	32.606	1.00 23.00	В
	ATOM ATOM	3175 3176	CD1 CD2		281	27.822	66.564	33.998	1.00 20.52	В
30	ATOM	3177	CE1		281	27.086	68.732	32.426	1.00 23.69	В
50	ATOM	3178	CE2		281	28.702	67.628	33.826	1.00 19.90	В
	ATOM	3179		PHE	281	28.328	68.718	33.038	1.00 22.07	В
	ATOM	3180		PHE	281	24.570	63.306	32.929	1.00 16.85	В
	ATOM	3181	0	PHE	281	23.370	63.589	32.962	1.00 17.22	В
35	MOTA	3182	N	SER	282	25.022	62.095	33.231	1.00 14.65	В
	ATOM	3183	H	SER	282	25.984	61.920	33.203	1.00 0.00 1.00 14.06	B B
	MOTA	3184	CA	SER	282 282	24.104 24.152	61.030 59.884	33.605 32.578	1.00 14.00	В
	MOTA	3185 3186	CB OG	SER SER	282	25.449	59.298	32.482	1.00 18.85	В
40	MOTA MOTA	3187	HG	SER	282	25.433	58.594	31.836	1.00 0.00	В
70	ATOM	3188	C	SER	282	24.449	60.516	34.984	1.00 15.44	В
	ATOM	3189	ō	SER	282	25.631	60.359	35.310	1.00 22.28	В
	ATOM	3190	N	ILE	283	23.413	60.278	35.787	1.00 16.47	В
	MOTA	3191	H	ILE	283	22.513	60.444	35.442	1.00 0.00	В
45	MOTA	3192	CA	ILE	283	23.541	59.776	37.152	1.00 12.03	В
	MOTA	3193	CB	ILE	283	22.870	60.730	38.164	1.00 13.63 1.00 11.53	B B
	MOTA	3194		ILE	283	22.863	60.095 62.072	39.532 38.237	1.00 18.66	В
	ATOM	3195	CG1		283 283	23.606 23.280	63.039	37.120	1.00 14.72	В
50	ATOM ATOM	3196 3197		ILE	283	22.842	58.403	37.283	1.00 20.66	В
50	ATOM	3198		ILE	283	21.623	58.291	37.068	1.00 19.36	В
	ATOM	3199		ALA	284	23.617	57.369	37.616	1.00 18.27	В
	MOTA	3200		ALA	284	24.579	57.514	37.731	1.00 0.00	В
	MOTA	3201		ALA	284	23.082	56.022	37.814	1.00 16.02	В
55	ATOM	3202	CB	ALA	284	24.000	54.974	37.196	1.00 17.51	В
	ATOM	3203		ALA	284	22.963	55.767	39.299	1.00 18.28	В
	ATOM	3204		ALA	284	23.956	55.892	40.018	1.00 22.88	В
	MOTA	3205		ILE	285	21.753	55.430	39.764 39.139	1.00 19.46 1.00 0.00	B B
<b>60</b>	MOTA	3206		ILE	285	21.001	55.378 55.137	41.182	1.00 0.00	В
60	ATOM	3207		ILE	285 285	21.523 20.188	55.716	41.703	1.00 20.10	В
	MOTA	3208 3209		ILE	285	19.893	55.174	43.103	1.00 17.01	В
	ATOM ATOM	3210			285	20.256	57.235	41.762	1.00 17.37	В
	ATOM	3211		ILE	285	19.131	57.923	41.023	1.00 18.02	В
65	ATOM	3212		ILE	285	21.469	53.621	41.280	1.00 20.23	В
05	ATOM	3213		ILE	285	20.615	52.986	40.659	1.00 20.26	В
	MOTA	3214		LEU	286	22.384	53.045	42.052	1.00 17.07	В
	ATOM	3215		LEU	286	23.012	53.610	42.549	1.00 0.00	В
	ATOM	3216		LEU	286	22.471	51.602	42.176	1.00 19.43	В
70	ATOM	3217		LEU	286	23.949	51.171	42.263	1.00 19.07	В
	ATOM	3218		LEU	286	25.035	51.649	41.276	1.00 17.49	В
	ATOM	3219		LEU	286	25.830	50.442	40.797 40.099	1.00 12.99 1.00 10.34	B B
	MOTA	3220	CD2	LEU	286	24.431	52.420	40.022	T.00 T0.34	ם

	ATOM	3221	С	LEU	286	21.722	51.058	43.382	1.00 21.59	В
	ATOM	3222	Ō	LEU	286	21.885	49.895	43.742	1.00 23.43	В
	ATOM	3223	N	GLY	287	20.899	51.903	43.997	1.00 21.97	В
	ATOM	3224	H	GLY	287	20.792	52.812	43.647	1.00 0.00	В
5	MOTA	3225	CA	GLY	287	20.158	51.493	45.173	1.00 19.38	В
-	MOTA	3226	С	GLY	287	19.312	50.236	45.051	1.00 23.15	В
	MOTA	3227	0	GLY	287	19.575	49.221	45.708	1.00 20.35	В
	MOTA	3228	N	HIS	288	18.285	50.308	44.215	1.00 17.51	В
	MOTA	3229	H	HIS	288	18.130	51.137	43.713	1.00 0.00	В
10	ATOM	3230	CA	HIS	288	17.387	49.196	44.027	1.00 14.47	В
	MOTA	3231	CB	HIS	288	16.298	49.571	43.042	1.00 14.52	В
	ATOM	3232	CG	HIS	288	15.289	48.495	42.825	1.00 15.66	В
	MOTA	3233	CD2	HIS	288	15.157	47.585	41.826	1.00 6.58	В
	ATOM	3234	ND1	HIS	288	14.289	48.220	43.731	1.00 10.26	В
15	ATOM	3235	HD1	HIS	288	14.116	48.715	44.551	1.00 0.00	В
	ATOM	3236	CE1		288	13.575	47.198	43.293	1.00 16.43	В
	MOTA	3237	NE2		288	14.083	46.794	42.141	1.00 11.36	В
	MOTA	3238	HE2		288	13.751	46.056	41.599	1.00 0.00	В
	MOTA	3239	C	HIS	288	18.086	47.939	43.532	1.00 20.49	В
20	MOTA	3240	0	HIS	288	17.786	46.833	43.982	1.00 21.10	В
	MOTA	3241	N	TYR	289	19.007	48.117	42.595	1.00 20.56	B B
	MOTA	3242	H	TYR	289	19.202	49.023	42.276	1.00 0.00	В
	ATOM	3243	CA	TYR	289	19.733	46.995	42.034	1.00 18.95 1.00 16.43	В
	MOTA	3244	CB	TYR	289	20.740	47.489	41.004	1.00 16.43	В
25	MOTA	3245	CG	TYR	289	20.221	47.446	39.597	1.00 16.33	В
	ATOM	3246		TYR	289	19.048	48.104	39.264 37.978	1.00 14.79	В
	MOTA	3247		TYR	289	18.563	48.086	38.592	1.00 23.30	В
	MOTA	3248		TYR	289	20.907 20.428	46.757 46.733	37.287	1.00 18.41	В
20	ATOM	3249		TYR	289 289	19.252	47.409	36.991	1.00 22.68	В
30	ATOM	3250	CZ	TYR	289	18.755	47.437	35.716	1.00 18.85	В
	MOTA	3251	OH	TYR TYR	289	17.943	47.954	35.703	1.00 0.00	В
	MOTA	3252 3253	HH	TYR	289	20.467	46.221	43.120	1.00 16.62	В
	MOTA	3254	C O	TYR	289	20.383	44.995	43.190	1.00 16.84	В
35	MOTA	3255	N	ASN	290	21.182	46.940	43.976	1.00 14.38	В
33	ATOM ATOM	3256	H	ASN	290	21.203	47.921	43.912	1.00 0.00	В
	ATOM	3257	CA	ASN	290	21.927	46.254	45.007	1.00 16.73	В
	ATOM	3258	CB	ASN	290	23.029	47.167	45.546	1.00 16.82	В
	ATOM	3259	CG	ASN	290	24.202	47.282	44.575	1.00 23.04	В
40	ATOM	3260		ASN	290	24.477	46.361	43.788	1.00 17.55	В
	ATOM	3261		ASN	290	24.892	48.410	44.618	1.00 21.77	В
	ATOM		HD21		290	24.637	49.116	45.247	1.00 0.00	В
	ATOM	3263	HD22		290	25.647	48.501	44.001	1.00 0.00	В
	ATOM	3264	С	ASN	290	21.016	45.733	46.110	1.00 18.43	В
45	ATOM	3265	0	ASN	290	21.301	44.698	46.720	1.00 15.23	В
	MOTA	3266	N	ARG	291	19.909	46.434	46.330	1.00 16.92	В
	MOTA	3267	H	ARG	291	19.744	47.244	45.805	1.00 0.00	В
	ATOM	3268	CA	ARG	291	18.926	46.034	47.336	1.00 21.23	В
	ATOM	3269	CB	ARG	291	17.804		47.452	1.00 24.15	В
50	MOTA	3270	CG	ARG	291	17.983	48.113	48.576	1.00 25.81	В
	ATOM	3271	CD	ARG	291	17.245	49.456	48.310	1.00 34.39	В
	ATOM	3272	ΝE	ARG	291	16.026	49.348	47.505	1.00 42.57	В
	$\mathbf{MOTA}$	3273	HE	ARG	291	15.575	48.480	47.481	1.00 0.00 1.00 43.67	B B
	ATOM	3274	CZ	ARG	291	15.478	50.349	46.806	1.00 43.67	В
55	MOTA	3275		ARG	291	16.035	51.551	46.803		В
	MOTA		HH11		291	16.864	51.719	47.331		В
	MOTA		HH12		291	15.620	52.293	46.275	1.00 0.00 1.00 39.35	В
	MOTA	3278		ARG	291	14.356	50.148	46.110 46.114	1.00 39.33	В
<b>60</b>	ATOM		HH21		291	13.920	49.248	45.585	1.00 0.00	В
60	ATOM		HH22		291	13.952	50.897	45.585	1.00 0.00	В
	ATOM	3281	C	ARG	291	18.337	44.690		1.00 10.17	В
	ATOM	3282	0	ARG	291	17.966	43.883	47.734	1.00 10.79	В
	MOTA	3283	N	GLY	292	18.283	44.442	45.607 44.967	1.00 18.23	В
<i>-</i> -	ATOM	3284		GLY	292	18.625	45.096	45.139	1.00 19.17	В
65	MOTA	3285		GLY	292	17.712	43.187		1.00 19.17	В
	MOTA	3286		GLY	292	18.625	42.170	44.468 43.759	1.00 20.74	В
	MOTA	3287	0	GLY	292	18.143	41.280 42.262	44.724	1.00 10.44	В
	ATOM	3288		ASN	293	19.925 20.235	42.262	44.724	1.00 19.28	В
70	ATOM	3289		ASN	293		42.945	44.101	1.00 23.38	В
70	ATOM	3290		ASN	293	20.918		44.101	1.00 21.82	В
	ATOM	3291		ASN	293	20.855	39.945 39.122	44.850	1.00 21.62	В
	ATOM	3292		ASN	293	22.109 22.011	39.122	43.727	1.00 20.89	В
	MOTA	3293	דמט	ASN	293	44.UII	JO. VAI	7J.141	1.00 20.00	

	MOTA	3294	ND2	ASN	293	23.286	39.667	44.580	1.00 16.64	В
	MOTA		HD21		293	23.321	40.544	45.016	1.00 0.00	В
			HD22		293	24.090	39.158	44.353	1.00 0.00	В
	ATOM					20.851	41.290	42.578	1.00 24.68	В
~	ATOM	3297		ASN	293				1.00 25.78	В
5	ATOM	3298		ASN	293	20.937	40.199	42.009		
	ATOM	3299	N	LEU	294	20.690	42.432	41.917	1.00 27.45	В
	ATOM	3300	H	LEU	294	20.582	43.268	42.415	1.00 0.00	В
	ATOM	3301	CA	LEU	294	20.666	42.454	40.457	1.00 26.46	В
	ATOM	3302	СВ	LEU	294	19.696	43.514	39.920	1.00 21.98	В
10	ATOM	3303		LEU	294	18.249	43.549	40.402	1.00 33.38	В
10	ATOM	3304	CD1		294	17.464	44.534	39.538	1.00 32.24	В
			CD2		294	17.639	42.177	40.334	1.00 27.44	В
	MOTA	3305					42.822	39.984	1.00 24.21	В
	MOTA	3306	C	LEU	294	22.063				В
	MOTA	3307	0	LEU	294	22.709	43.685	40.571	1.00 23.66	
15	MOTA	3308	N	SER	295	22.526	42.174	38.924	1.00 23.08	В
	ATOM	3309	H	SER	295	21.984	41.469	38.512	1.00 0.00	В
	ATOM	3310	CA	SER	295	23.833	42.497	38.366	1.00 24.49	В
	MOTA	3311	CB	SER	295	24.211	41.481	37.284	1.00 22.71	В
	ATOM	3312	OG	SER	295	25.057	42.058	36.307	1.00 28.77	В
20	ATOM	3313	HG	SER	295	25.856	42.370	36.726	1.00 0.00	В
20		3314	C	SER	295	23.724	43.909	37.759	1.00 20.29	В
	ATOM					22.815	44.187	36.983	1.00 18.00	В
	ATOM	3315	0	SER	295			38.118	1.00 16.49	В
	ATOM	3316	N	THR	296	24.660	44.777			В
	MOTA	3317	H	THR	296	25.372	44.479	38.724	1.00 0.00	
25	ATOM	3318	CA	THR	296	24.679	46.166	37.653	1.00 18.66	В
	MOTA	3319	CB	THR	296	25.023	47.101	38.804	1.00 19.68	В
	MOTA	3320	OG1	THR	296	26.258	46.675	39.393	1.00 19.06	В
	MOTA	3321	HG1	THR	296	26.162	45.778	39.722	1.00 0.00	В
	ATOM	3322		THR	296	23.927	47.060	39.863	1.00 22.45	В
30		3323	C	THR	296	25.664	46.470	36.535	1.00 19.63	В
30	ATOM				296	25.808	47.626	36.136	1.00 17.70	В
	ATOM	3324	0	THR			45.439	36.016	1.00 21.20	В
	MOTA	3325	N	GLU	297	26.324			1.00 21.20	В
	ATOM	3326	H	GLU	297	26.131	44.536	36.341		
	MOTA	3327	CA	GLU	297	27.325	45.622	34.972	1.00 21.26	В
35	MOTA	3328	CB	$\operatorname{GLU}$	297	28.042	44.291	34.710	1.00 30.39	В
	ATOM	3329	CG	GLU	297	29.004	43.863	35.838	1.00 39.46	В
	ATOM	3330	CD	GLU	297	28.305	43.191	37.015	1.00 41.75	В
	ATOM	3331		GLU	297	27.330	42.455	36.778	1.00 45.39	В
	ATOM	3332		GLU	297	28.735	43.392	38.173	1.00 35.85	В
40		3333	C	GLU	297	26.789	46.210	33.675	1.00 22.11	В
40	MOTA				297	27.344	47.184	33.151	1.00 18.94	В
	MOTA	3334		GLU			45.622	33.153	1.00 15.26	В
	MOTA	3335		LYS	298	25.717			1.00 13.20	В
	MOTA	3336		LYS	298	25.330	44.845	33.608		
	MOTA	3337	CA	LYS	298	25.105	46.107	31.925	1.00 17.69	В
45	MOTA	3338	CB	LYS	298	23.958	45.163	31.500	1.00 22.54	В
	MOTA	3339	CG	LYS	298	23.297	45.486	30.151	1.00 16.04	В
	ATOM	3340	CD	LYS	298	22.093	44.565	29.903	1.00 15.19	В
	ATOM	3341	CE	LYS	298	21.795	44.409	28.415	1.00 24.32	В
	ATOM	3342		LYS	298	20.353	44.064	28.147	1.00 31.08	В
50	ATOM	3343		LYS	298	19.741	44.822	28.518	1.00 0.00	В
50	ATOM	3344		LYS	298	20.114	43.169	28.620	1.00 0.00	В
				LYS	298	20.202	43.968	27.124	1.00 0.00	В
	ATOM	3345				24.556	47.506	32.172	1.00 14.71	В
	MOTA	3346		LYS	298				1.00 19.72	В
	ATOM	3347		LYS	298	24.718	48.410	31.356		
55	ATOM	3348	N	PHE	299	23.915	47.659	33.322	1.00 19.20	В
	MOTA	3349	H	PHE	299	23.860	46.891	33.929	1.00 0.00	В
	ATOM	3350	CA	PHE	299	23.283	48.912	33.744	1.00 16.23	В
	ATOM	3351	. CB	PHE	299	22.600	48.673	35.110	1.00 15.69	В
	ATOM	3352		PHE	299	22.135	49.920	35.826	1.00 17.83	В
60	ATOM	3353		PHE	299	21.724	51.058	35.127	1.00 17.90	В
00					299	22.110	49.949	37.216	1.00 17.55	В
	MOTA	3354		PHE			52.191	35.802	1.00 15.38	B
	MOTA	3355		PHE	299	21.303			1.00 26.58	В
	MOTA	3356		PHE	299	21.687	51.087	37.897		
	MOTA	3357		PHE	299	21.282	52.213	37.179	1.00 19.56	В
65	MOTA	3358	C	PHE	299	24.276	50.079	33.818	1.00 17.61	В
	MOTA	3359		PHE	299	24.087	51.099	33.163	1.00 16.95	В
	ATOM	3360		VAL	300	25.327	49.914	34.617	1.00 17.22	В
	ATOM	3361		VAL	300	25.433	49.066	35.094	1.00 0.00	В
		3362		VAL	300	26.322	50.959	34.801	1.00 18.55	В
70	ATOM				300	27.421	50.492	35.773	1.00 16.60	В
70	ATOM	3363		VAL			51.220	35.492	1.00 21.52	В
	ATOM	3364		VAL	300	28.724			1.00 21.32	В
	MOTA	3365		VAL	300	26.974	50.723	37.195		
	MOTA	3366	5 C	VAL	300	26.941	51.382	33.480	1.00 17.23	В

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	MOTA	3367	0	VAL	300	27.075	52.569	33.198	1.00 15.55 1.00 15.45	B B
	MOTA	3368	N	GLU	301	27.293	50.400 49.471	32.665 32.939	1.00 13.43	В
	ATOM	3369	H	GLU	301	27.145 27.892	50.674	31.374	1.00 0.00	В
5	ATOM	3370	CA	GLU	301 301	28.282	49.349	30.708	1.00 25.34	В
3	MOTA	3371 3372	CB CG	GLU GLU	301	28.738	49.477	29.274	1.00 40.60	B
	MOTA	3372	CD	GLU	301	27.589	49.413	28.283	1.00 50.61	В
	MOTA	3374	OE1		301	26.510	48.871	28.633	1.00 56.16	В
	ATOM	3375		GLU	301	27.771	49.908	27.146	1.00 54.98	В
10	MOTA MOTA	3376	C	GLU	301	26.956	51.483	30.457	1.00 22.33	В
10	ATOM	3377	0	GLU	301	27.413	52.316	29.663	1.00 18.68	В
	ATOM	3378	N	GLU	302	25.652	51.235	30.573	1.00 21.56	В
	ATOM	3379	Н	GLU	302	25.349	50.566	31.221	1.00 0.00	В
	ATOM	3380	CA	GLU	302	24.655	51.931	29.759	1.00 19.52	В
15	ATOM	3381	CB	GLU	302	23.316	51.173	29.825	1.00 23.59	В
15	MOTA	3382	CG	GLU	302	22.069	51.902	29.281	1.00 26.77	В
	ATOM	3383	CD	GLU	302	20.820	51.024	29.367	1.00 19.66	В
	ATOM	3384	OE1	GLU	302	20.836	49.919	28.798	1.00 15.94	В
	MOTA	3385	OE2	GLU	302	19.836	51.428	30.010	1.00 19.29	В
20	ATOM	3386	С	GLU	302	24.487	53.409	30.163	1.00 13.52	В
	ATOM	3387	0	GLU	302	24.426	54.276	29.303	1.00 17.34	В
	ATOM	3388	N	ILE	303	24.419	53.710	31.452	1.00 17.66	В
	MOTA	3389	H	ILE	303	24.459	53.009	32.135	1.00 0.00	В
	ATOM	3390	CA	ILE	303	24.282	55.117	31.825	1.00 15.73	В
25	ATOM	3391	CB	ILE	303	24.030	55.310	33.330	1.00 18.32	В
	MOTA	3392	CG2	ILE	303	23.348	56.686	33.566	1.00 12.98	В
	MOTA	3393	CG1	ILE	303	23.163	54.164	33.864	1.00 21.47	В
	MOTA	3394	CD1	$_{ m ILE}$	303	21.731	54.137	33.322	1.00 24.44	В
	MOTA	3395	С	$_{ m ILE}$	303	25.575	55.848	31.452	1.00 20.62	В
30	ATOM	3396	0	ILE	303	25.542	57.005	31.051	1.00 22.42	B B
	MOTA	3397	N	LYS	304	26.715	55.172	31.593 31.932	1.00 17.68 1.00 0.00	В
	MOTA	3398	H	LYS	304	26.703	54.253 55.805	31.236	1.00 0.00	В
	MOTA	3399	CA	LYS	304	27.980 29.183	54.907	31.236	1.00 22.31	В
25	ATOM	3400	CB	LYS LYS	304 304	30.528	55.611	31.424	1.00 27.58	В
35	MOTA	3401 3402	CG CD	LYS	304	31.449	55.355	32.617	1.00 29.45	В
	MOTA MOTA	3402	CE	LYS	304	32.745	56.172	32.533	1.00 33.25	В
	ATOM	3404	NZ	LYS	304	33.272	56.638	33.870	1.00 32.84	В
	MOTA	3405		LYS	304	33.470	55.816	34.473	1.00 0.00	В
40	ATOM	3406		LYS	304	32.561	57.243	34.330	1.00 0.00	В
10	ATOM	3407		LYS	304	34.147	57.184	33.727	1.00 0.00	В
	ATOM	3408	C	LYS	304	27.963	56.096	29.745	1.00 20.33	В
	MOTA	3409	Ō	LYS	304	28.455	57.130	29.307	1.00 21.96	В
	MOTA	3410	N	SER	305	27.376	55.185	28.977	1.00 16.80	В
45	ATOM	3411	H	SER	305	26.990	54.387	29.393	1.00 0.00	В
	MOTA	3412	CA	SER	305	27.295	55.346	27.534	1.00 20.13	В
	MOTA	3413	CB	SER	305	26.662	54.112	26.898	1.00 18.58	В
	ATOM	3414	OG	SER	305	25.453	54.454	26.253	1.00 30.77	В
	MOTA	3415	$^{\mathrm{HG}}$	SER	305	25.630	55.103	25.567	1.00 0.00	В
50	ATOM	3416	C	SER	305	26.517	56.584	27.107	1.00 15.70	В
	MOTA	3417	0	SER	305	26.679	57.045	25.991	1.00 14.73	В
	ATOM	3418	N	ILE	306	25.677	57.110	27.994	1.00 20.28	В
	ATOM	3419	H	ILE	306	25.593	56.689	28.877	1.00 0.00 1.00 14.20	B B
سر س	ATOM	3420	CA	ILE	306	24.872	58.299 58.269	27.698 28.527	1.00 14.20	В
55	MOTA	3421	CB	ILE	306	23.555 22.895	59.661	28.591	1.00 23.10	В
	ATOM	3422		ILE	306	22.588	57.265	27.900	1.00 23.41	В
	MOTA	3423	CG1	ILE	306 306	22.204	56.151	28.834	1.00 19.11	В
	ATOM	3424 3425		ILE	306	25.656	59.594	27.985	1.00 18.43	В
60	ATOM ATOM	3425	С 0	ILE	306	25.481	60.596	27.301	1.00 15.22	В
00	ATOM	3427	N	ALA	307	26.522	59.555	28.996	1.00 20.05	В
	ATOM	3428	H	ALA	307	26.607	58.727	29.512	1.00 0.00	В
	ATOM	3429	CA	ALA	307	27.350	60.711	29.369	1.00 21.87	В
	MOTA	3430	CB	ALA	307	28.291	60.341	30.515	1.00 13.67	В
65	ATOM	3431	C	ALA	307	28.177	61.271	28.226	1.00 15.95	В
0.5	ATOM	3432	Õ	ALA	307	28.653	60.542	27.370	1.00 18.44	В
	MOTA	3433	N	SER	308	28.343	62.583	28.231	1.00 18.17	В
	ATOM	3434	H	SER	308	27.907	63.117	28.925	1.00 0.00	В
	ATOM	3435	CA	SER	308	29.154	63.252	27.225	1.00 19.58	В
70	ATOM	3436	CB	SER	308	28.962	64.759	27.306	1.00 15.23	В
	ATOM	3437	QG	SER	308	27.810	65.168	26.610	1.00 22.22	В
	MOTA	3438	HG	SER	308	27.890	64.920	25.685	1.00 0.00	В
	ATOM	3439	C	SER	308	30.606	62.935	27.556	1.00 16.69	В

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	ATOM	3440	O SER	308	30.930 31.478	62.608 63.027	28.691 26.570	1.00 19.32 1.00 19.87	B B
	MOTA MOTA	3441 3442	N GLU H GLU	309 309	31.181	63.264	25.667	1.00 13.07	В
	MOTA	3443	CA GLU	309	32.883	62.772	26.840	1.00 27.15	В
5	MOTA	3444	CB GLU	309	33.576	62.254	25.586	1.00 30.43	В
Ū	ATOM	3445	CG GLU	309	33.735	60.743	25.594	1.00 42.04	В
	MOTA	3446	CD GLU	309	33.305	60.100	24.293	1.00 51.38	В
	MOTA	3447	OE1 GLU	309	33.438	58.860	24.165	1.00 53.41	В
1.0	MOTA	3448	OE2 GLU	309	32.836	60.835	23.398	1.00 53.07	B B
10	ATOM	3449	C GLU	309	33.549 33.260	64.049 65.147	27.339 26.859	1.00 23.13 1.00 24.83	В
	MOTA	3450 3451	O GLU N PRO	309 310	34.429	63.934	28.339	1.00 22.49	В
	ATOM ATOM	3452	CD PRO	310	35.090	65.153	28.838	1.00 22.94	B
	ATOM	3453	CA PRO	310	34.873	62.730	29.061	1.00 20.46	В
15	MOTA	3454	CB PRO	310	36.043	63.238	29.899	1.00 21.98	В
	ATOM	3455	CG PRO	310	35.744	64.692	30.108	1.00 22.65	В
	MOTA	3456	C PRO	310	33.789	62.122	29.952	1.00 20.72	В
	ATOM	3457	O PRO	310	33.170	62.840	30.748	1.00 21.32	В
20	ATOM	3458	N THR	311	33.557	60.813	29.833 29.184	1.00 16.53 1.00 0.00	B B
20	MOTA	3459	H THR CA THR	311 311	34.066 32.556	60.282 60.172	30.669	1.00 20.30	В
	MOTA MOTA	3460 3461	CB THR	311	32.387	58.671	30.367	1.00 26.73	В
	ATOM	3462	OG1 THR	311	33.656	58.018	30.481	1.00 33.48	В
	ATOM	3463	HG1 THR	311	33.997	58.128	31.371	1.00 0.00	В
25	MOTA	3464	CG2 THR	311	31.798	58.449	28.983	1.00 27.71	В
	MOTA	3465	C THR	311	32.894	60.277	32.153	1.00 25.27	В
	MOTA	3466	O THR	311	32.022	60.561	32.960	1.00 29.95	В
	ATOM	3467	N GLU	312	34.153 34.837	60.052 59.854	32.524 31.852	1.00 24.13	B B
30	MOTA MOTA	3468 3469	H GLU CA GLU	312 312	34.509	60.104	33.940	1.00 27.24	В
30	ATOM	3470	CB GLU	312	36.004	59.840	34.153	1.00 30.20	В
	MOTA	3471	CG GLU	312	36.889	60.121	32.953	1.00 44.57	В
	MOTA	3472	CD GLU	312	36.932	58.966	31.967	1.00 42.06	В
	MOTA	3473	OE1 GLU	312	37.286	57.844	32.376	1.00 44.27	В
35	MOTA	3474	OE2 GLU	312	36.609	59.188	30.778	1.00 45.67	В
	ATOM	3475	C GLU	312	34.116	61.425	34.590 35.803	1.00 28.79 1.00 25.09	B B
	MOTA	3476	O GLU N LYS	312 313	33.898 34.028	61.483 62.485	33.795	1.00 25.03	В
	ATOM ATOM	3477 3478	N LYS H LYS	313	34.229	62.399	32.840	1.00 0.00	В
40	MOTA	3479	CA LYS	313	33.635	63.776	34.340	1.00 24.40	В
, ,	ATOM	3480	CB LYS	313	34.311	64.904	33.563	1.00 29.52	В
	ATOM	3481	CG LYS	313	35.760	65.150	33.989	1.00 40.92	В
	MOTA	3482	CD LYS	313	35.838	66.011	35.246	1.00 42.61	В
15	MOTA	3483	CE LYS	313	37.263	66.454	35.516 36.668	1.00 44.08 1.00 45.93	B B
45	ATOM ATOM	3484 3485	NZ LYS HZ1 LYS	313 313	37.340 36.977	67.390 66.918	37.522	1.00 43.33	В
	ATOM	3486	HZ1 LYS	313	36.767	68.234	36.469	1.00 0.00	В
	ATOM	3487	HZ3 LYS	313	38.329	67.670	36.822	1.00 0.00	В
	ATOM	3488	C LYS	313	32.114	63.968	34.305	1.00 23.67	В
50	ATOM	3489	O LYS	313	31.546	64.615	35.183	1.00 21.16	В
	ATOM	3490	N HIS	314	31.462	63.394	33.299	1.00 17.77	В
	ATOM	3491	H HIS	314	31.956 30.026	62.860 63.546	32.643 33.163	1.00 0.00 1.00 23.14	B B
	ATOM	3492 3493	CA HIS CB HIS	314 314	29.664	63.688	31.681	1.00 23.14	В
55	MOTA ATOM	3494	CG HIS	314	30.242	64.916	31.035	1.00 26.47	В
55	ATOM	3495	CD2 HIS	314	31.317	65.073	30.226	1.00 24.55	В
	MOTA	3496	ND1 HIS	314	29.652	66.157	31.136	1.00 27.43	В
	MOTA	3497	HD1 HIS	314	28.867	66.359	31.682	1.00 0.00	В
	MOTA	3498	CE1 HIS	314	30.344	67.031	30.426	1.00 13.83	В
60	MOTA	3499	NE2 HIS	314	31.355	66.398 66.817	29.864	1.00 30.72 1.00 0.00	B B
	ATOM	3500	HE2 HIS	314 314	32.021 29.178	62.430	29.289 33.812	1.00 0.00 1.00 19.97	В
	ATOM ATOM	3501 3502	C HIS	314	28.022	62.663	34.133	1.00 15.17	В
	ATOM	3502	N PHE	315	29.752	61.245	34.019	1.00 12.58	В
65	ATOM	3504	H PHE	315	30.680	61.109	33.753	1.00 0.00	В
	MOTA	3505	CA PHE	315	29.018	60.139	34.637	1.00 11.72	В
	MOTA	3506	CB PHE	315	29.435	58.799	34.022	1.00 13.63	В
	ATOM	3507	CG PHE	315	28.821	57.595	34.702	1.00 17.15	В
70	ATOM	3508	CD1 PHE	315	27.427	57.409	34.716 35.320	1.00 12.18 1.00 21.49	В В
70	ATOM	3509 3510	CD2 PHE CE1 PHE	315 315	29.626 26.856	56.635 56.290	35.320	1.00 21.49	В
	ATOM ATOM	3510	CE1 PHE	315	29.052	55.501	35.941	1.00 19.73	В
	ATOM	3512	CZ PHE	315	27.651	55.337	35.943	1.00 11.10	В
		~ <del>-</del>							

					24.5	00 100	60 015	26 152	1 00 00 05	_
	ATOM ATOM	3513 3514	C 0	PHE PHE	315 315	29.189 30.307	60.045 60.141	36.153 36.672	1.00 20.36 1.00 18.84	B B
	ATOM	3515	N	PHE	316	28.074	59.844	36.863	1.00 23.38	В
_	MOTA	3516	H	PHE	316	27.214	59.795	36.398	1.00 0.00	В
5	ATOM	3517	CA	PHE	316	28.107	59.697	38.317	1.00 14.23	В
	ATOM ATOM	3518 3519	CB CG	PHE PHE	316 316	27.395 28.065	60.853 62.188	39.002 38.810	1.00 19.22 1.00 27.88	B B
	ATOM	3520	CD1		316	27.744	62.994	37.721	1.00 28.03	В
	ATOM	3521	CD2		316	28.969	62.675	39.754	1.00 31.78	В
10	MOTA	3522	CE1		316	28.306	64.271	37.578	1.00 29.90	В
	MOTA	3523	CE2 CZ	PHE	316 316	29.535 29.195	63.959 64.746	39.609 38.523	1.00 25.22 1.00 25.24	B B
	MOTA MOTA	3524 3525	C	PHE	316	27.453	58.392	38.737	1.00 23.24	В
	MOTA	3526	Õ	PHE	316	26.306	58.100	38.370	1.00 16.18	В
15	MOTA	3527	N	ASN	317	28.194	57.593	39.489	1.00 22.70	В
	ATOM	3528	H	ASN	317	29.106	57.868 56.312	39.725 39.979	1.00 0.00 1.00 23.24	B B
	ATOM ATOM	3529 3530	CA CB	ASN ASN	317 317	27.695 28.741	55.210	39.759	1.00 23.24	В
	ATOM	3531	CG	ASN	317	28.335	53.871	40.391	1.00 25.87	В
20	ATOM	3532		ASN	317	27.738	53.828	41.467	1.00 26.08	В
	MOTA	3533	ND2		317	28.658	52.778	39.716	1.00 13.17	В
	ATOM ATOM		HD21 HD22		317 317	29.130 28.407	52.855 51.916	38.858 40.103	1.00 0.00 1.00 0.00	B B
	ATOM	3536	C	ASN	317	27.410	56.484	41.463	1.00 18.96	В
25	ATOM	3537	Ö	ASN	317	28.326	56.476	42.277	1.00 21.45	В
	ATOM	3538	N	VAL	318	26.142	56.669	41.804	1.00 23.81	В
	ATOM	3539 3540	H CA	VAL VAL	318 318	25.458 25.731	56.678 56.857	41.102 43.187	1.00 0.00 1.00 20.00	B B
	ATOM ATOM	3541	CB	VAL	318	24.576	57.902	43.272	1.00 20.00	В
30	ATOM	3542		VAL	318	23.466	57.514	42.335	1.00 27.34	В
	MOTA	3543		VAL	318	24.060	58.012	44.688	1.00 15.43	В
	MOTA MOTA	35 <b>44</b> 35 <b>4</b> 5	C	VAL VAL	318 318	25.280 24.488	55.508 54.814	43.737 43.108	1.00 20.44 1.00 17.67	B B
	ATOM	3546	И	SER	319	25.797	55.133	44.903	1.00 20.29	В
35	MOTA	3547	Н	SER	319	26.417	55.731	45.369	1.00 0.00	В
	ATOM	3548	CA	SER	319	25.455	53.840	45.502	1.00 17.71	В
	ATOM ATOM	3549 3550	CB OG	SER SER	319 319	26.268 27.123	53.608 54.701	46.775 47.038	1.00 13.81 1.00 31.29	B B
	ATOM	3551	HG	SER	319	26.599	55.496	47.151	1.00 0.00	В
40	MOTA	3552	С	SER	319	23.969	53.697	45.816	1.00 18.64	В
	MOTA	3553	0	SER	319	23.382	52.644	45.575	1.00 16.85	B B
	ATOM ATOM	3554 3555	N H	ASP ASP	320 320	23.361 23.866	54.745 55.566	46.351 46.537	1.00 16.38 1.00 0.00	В
	ATOM	3556	CA	ASP	320	21.943	54.679	46.665	1.00 20.08	В
45	ATOM	3557	CB	ASP	320	21.720	53.772	47.878	1.00 26.71	В
	ATOM	3558	CG	ASP	320	22.310	54.337	49.143	1.00 23.52 1.00 27.09	B B
	ATOM ATOM	3559 3560		ASP ASP	320 320	23.287 21.791	55.104 54.013	49.059 50.227	1.00 27.09	В
	MOTA	3561		ASP	320	21.317		46.886	1.00 16.45	В
50	MOTA	3562	0	ASP	320	22.018	57.062	47.037	1.00 15.80	В
	ATOM	3563		GLU	321	19.991	56.088	46.902	1.00 14.19 1.00 0.00	B B
	MOTA MOTA	3564 3565	H CA	GLU GLU	321 321	19.508 19.220	55.238 57.313	46.818 47.037	1.00 0.00	В
	MOTA	3566	CB	GLU	321	17.738	56.966	47.233	1.00 12.70	В
55	MOTA	3567	CG	GLU	321	17.115	56.285	46.017	1.00 12.53	В
	ATOM	3568	CD	GLU	321	17.187	54.767	46.098	1.00 17.82 1.00 14.77	В В
	ATOM ATOM	3569 3570		GLU GLU	321 321	17.982 16.439	54.231 54.103	46.903 45.355	1.00 14.77	В
	ATOM	3571	C	GLU	321	19.675	58.272	48.130	1.00 24.90	В
60	ATOM	3572	0	GLU	321	19.749	59.480	47.906	1.00 22.58	В
	MOTA	3573	N	LEU	322	19.967	57.732	49.307	1.00 26.45 1.00 0.00	B B
	MOTA ATOM	3574 3575	H CA	LEU LEU	322 322	19.881 20.411	56.763 58.550	49.428 50.425	1.00 0.00	В
	ATOM	3576	CB	LEU	322	20.411	57.707	51.709	1.00 32.06	В
65	MOTA	3577	CG	LEU	322	19.155	57.600	52.478	1.00 34.11	В
	ATOM	3578		LEU	322	19.357	56.923	53.839	1.00 29.26	В
	ATOM	3579 3580		LEU LEU	322 322	18.583 21.768	59.000 59.193	52.645 50.154	1.00 30.30 1.00 30.66	B B
	ATOM ATOM	3580		LEU	322	22.119	60.195	50.776	1.00 33.88	В
70	ATOM	3582	N	ALA	323	22.527	58.625	49.219	1.00 26.52	В
	ATOM	3583		ALA	323	22.199	57.828	48.752	1.00 0.00	В
	ATOM	3584		ALA	323 323	23.839 24.772	59.166 58.030	48.886 48.451	1.00 24.47 1.00 19.17	B B
	MOTA	3585	CD	ALA	263	47.114	20.020	40.401	1.00 1J.1/	ב

	MOTA	3586	C ALA	323	23.832	60.283	47.820	1.00 24.00	В
	MOTA	3587	O ALA	323	24.829	60.971	47.657	1.00 24.66	В
	ATOM	3588	N LEU	324	22.735	60.481	47.096	1.00 21.81	В
5	ATOM	3589 3590	H LEU	324 324	21.941 22.715	59.928 61.534	47.248 46.069	1.00 0.00 1.00 19.68	B B
5	ATOM ATOM	3591	CA LEU CB LEU	324	21.312	61.715	45.508	1.00 19.00	В
	ATOM	3592	CG LEU	324	20.899	60.637	44.519	1.00 13.78	В
	ATOM	3593	CD1 LEU	324	19.402	60.611	44.457	1.00 16.65	В
	ATOM	3594	CD2 LEU	324	21.511	60.908	43.143	1.00 14.31	В
10	MOTA	3595	C LEU	324	23.226	62.892	46.561	1.00 23.65	В
	MOTA	3596	O LEU	324	23.938	63.594	45.841	1.00 18.23	В
	ATOM	3597	N VAL	325	22.852	63.264	47.783	1.00 26.30	В
	MOTA	3598	H VAL	325 325	22.272 23.282	62.672 64.533	48.305 48.369	1.00 0.00 1.00 31.91	B B
15	MOTA MOTA	3599 3600	CA VAL CB VAL	325	22.778	64.643	49.837	1.00 31.31	В
13	ATOM	3601	CG1 VAL	325	23.583	65.687	50.609	1.00 34.83	В
	ATOM	3602	CG2 VAL	325	21.294	65.008	49.843	1.00 42.56	В
	ATOM	3603	C VAL	325	24.819	64.710	48.330	1.00 30.26	В
	MOTA	3604	O VAL	325	25.327	65.825	48.398	1.00 32.04	В
20	ATOM	3605	N THR	326	25.548	63.609	48.194	1.00 28.75	В
	ATOM	3606	H THR	326	25.094 26.998	62.744 63.657	48.113 48.167	1.00 0.00 1.00 31.17	B B
	ATOM ATOM	3607 3608	CA THR	326 326	27.607	62.288	48.511	1.00 31.17	В
	ATOM	3609	OG1 THR	326	27.229	61.332	47.514	1.00 34.82	В
25	ATOM	3610	HG1 THR	326	26.277	61.260	47.489	1.00 0.00	В
	ATOM	3611	CG2 THR	326	27.136	61.826	49.880	1.00 30.51	В
	MOTA	3612	C THR	326	27.608	64.128	46.856	1.00 32.05	В
	MOTA	3613	O THR	326	28.745	64.590	46.846	1.00 30.58	В
20	ATOM	3614	N ILE	327	26.879 25.984	64.002 63.603	45.750 45.793	1.00 33.07 1.00 0.00	B B
30	ATOM ATOM	3615 3616	H ILE CA ILE	327 327	27.421	64.461	44.472	1.00 0.00	В
	ATOM	3617	CB ILE	327	27.185	63.446	43.300	1.00 35.01	В
	ATOM	3618	CG2 ILE	327	27.881	62.118	43.604	1.00 32.57	В
	MOTA	3619	CG1 ILE	327	25.691	63.252	43.048	1.00 35.05	В
35	ATOM	3620	CD1 ILE	327	25.371	62.796	41.633	1.00 32.92	В
	ATOM	3621	C ILE	327	26.852	65.814	44.061	1.00 30.01	B B
	MOTA	3622 3623	O ILE N VAL	327 328	27.211 25.972	66.348 66.370	43.011 44.894	1.00 23.73 1.00 26.90	В
	ATOM ATOM	3624	N VAL H VAL	328	25.715	65.896	45.711	1.00 20.90	В
40	ATOM	3625	CA VAL	328	25.383	67.675	44.600	1.00 32.68	В
	ATOM	3626	CB VAL	328	24.535	68.177	45.798	1.00 36.74	В
	MOTA	3627	CG1 VAL	328	24.075	69.612	45.561	1.00 29.92	В
	ATOM	3628	CG2 VAL	328	23.332	67.265	45.998	1.00 30.30	В
45	ATOM	3629	C VAL	328	26.451 26.310	68.741 69.477	44.255 43.279	1.00 33.15 1.00 35.10	B B
43	ATOM ATOM	3630 3631	O VAL N LYS	328 329	27.528	68.801	45.038	1.00 33.10	В
	ATOM	3632	H LYS	329	27.613	68.169	45.781	1.00 0.00	В
	ATOM	3633	CA LYS	329	28.585	69.789	44.819	1.00 31.42	В
	MOTA	3634	CB LYS	329	29.563	69.773	45.990	1.00 38.34	В
50	MOTA	3635	CG LYS	329	29.794	71.139	46.623	1.00 42.75	В
	ATOM	3636	CD LYS	329	29.245 27.716	71.201 71.275	48.053 48.078	1.00 46.58 1.00 48.13	B B
	ATOM ATOM	3637 3638	CE LYS NZ LYS	329 329	27.716	70.078	48.711	1.00 48.13	В
	ATOM	3639	HZ1 LYS	329	27.420	69.992	49.693	1.00 0.00	В
55	ATOM	3640	HZ2 LYS	329	27.357	69.225	48.180	1.00 0.00	В
	ATOM	3641	HZ3 LYS	329	26.055	70.182	48.701	1.00 0.00	В
	MOTA	3642	C LYS	329	29.365	69.648	43.517	1.00 29.75	В
	MOTA	3643	O LYS	329	29.548	70.633	42.791	1.00 30.62	В
40	MOTA	3644	N ALA	330	29.818 29.623	68.434 67.699	43.226 43.844	1.00 27.05 1.00 0.00	В В
60	ATOM ATOM	36 <b>4</b> 5 36 <b>4</b> 6	H ALA CA ALA	330 330	30.598	68.145	42.022	1.00 27.52	В
	ATOM	3647	CB ALA	330	31.094	66.683	42.058	1.00 15.14	В
	ATOM	3648	C ALA	330	29.804	68.397	40.742	1.00 24.45	В
	ATOM	3649	O ALA	330	30.282	69.043	39.811	1.00 29.53	В
65	MOTA	3650	N LEU	331	28.585	67.878	40.708	1.00 27.74	В
	ATOM	3651	H LEU	331	28.266	67.372	41.483	1.00 0.00	В
	MOTA	3652	CA LEU	331	27.701	68.040 67.267	39.555 39.771	1.00 26.77 1.00 20.69	В В
	ATOM ATOM	3653 3654	CB LEU	331 331	26.398 25.594	66.834	39.771	1.00 20.69	В
70	ATOM	3655	CD1 LEU	331	24.126	67.117	38.817	1.00 32.10	В
, 5	ATOM	3656	CD2 LEU	331	26.079	67.540	37.280	1.00 22.24	В
	MOTA	3657	C LEU	331	27.358	69.497	39.326	1.00 14.45	В
	MOTA	3658	O LEU	331	27.376	69.973	38.209	1.00 25.05	В

	MOTA	3659	N	GLY	332	27.036	70.199	40.400	1.00 20.98	В
	MOTA	3660	H	GLY	332	27.036	69.772	41.280	1.00 0.00	В
	ATOM	3661	CA	GLY	332	26.683	71.599	40.277	1.00 16.97	В
	MOTA	3662	C	GLY	332	27.830	72.431	39.740	1.00 23.19	В
5	MOTA	3663	Ö	GLY	332	27.611	73.389	39.000	1.00 20.06	В
•	ATOM	3664	N	GLU	333	29.063	72.086	40.102	1.00 22.14	В
	ATOM	3665	H	GLU	333	29.218	71.324	40.699	1.00 0.00	В
	MOTA	3666	CA	GLU	333	30.169	72.870	39.589	1.00 28.24	В
	ATOM	3667	CB	GLU	333	31.358	72.859	40.557	1.00 28.24	В
10					333	31.779	71.505	41.068	1.00 40.29	В
10	ATOM	3668	CG	GLU			71.505			
	ATOM	3669	CD	GLU	333	33.065		41.866	1.00 46.24	В
	ATOM	3670	OE1		333	34.122	71.152	41.350	1.00 45.00	В
	MOTA	3671	OE2		333	33.008	72.121	43.006	1.00 38.74	В
1.5	MOTA	3672	C	GLU	333	30.594	72.407	38.206	1.00 27.85	В
15	MOTA	3673	0	GLU	333	31.048	73.215	37.397	1.00 29.71	В
	MOTA	3674	N	ARG	334	30.438	71.115	37.920	1.00 25.03	В
	MOTA	3675	H	ARG	334	30.079	70.508	38.601	1.00 0.00	В
	MOTA	3676	CA	ARG	334	30.799	70.594	36.602	1.00 18.82	В
	MOTA	3677	CB	ARG	334	30.839	69.062	36.610	1.00 17.45	В
20	MOTA	3678	CG	ARG	334	32.187	68.485	36.951	1.00 12.28	В
	MOTA	3679	CD	ARG	334	32.112	66.986	37.157	1.00 20.12	В
	MOTA	3680	NE	ARG	334	33.151	66.520	38.065	1.00 26.33	В
	MOTA	3681	$_{ m HE}$	ARG	334	33.835	67.163	38.343	1.00 0.00	В
	MOTA	3682	CZ	ARG	334	33.230	65.281	38.543	1.00 33.67	В
25	MOTA	3683	NH1	ARG	334	32.321	64.366	38.200	1.00 28.50	В
	MOTA	3684	HH11	ARG	334	31.575	64.611	37.583	1.00 0.00	В
	ATOM	3685	HH12	ARG	334	32.388	63.437	38.563	1.00 0.00	В
	ATOM	3686	NH2	ARG	334	34.220	64.956	39.364	1.00 33.01	В
	MOTA	3687	HH21	ARG	334	34.901	65.642	39.624	1.00 0.00	В
30	ATOM	3688	HH22	ARG	334	34.287	64.026	39.728	1.00 0.00	В
	ATOM	3689	C	ARG	334	29.811	71.057	35.532	1.00 16.42	В
	ATOM	3690	0	ARG	334	30.185	71.277	34.383	1.00 17.09	В
	MOTA	3691	N	ILE	335	28.541	71.184	35.889	1.00 18.26	В
	MOTA	3692	Н	ILE	335	28.256	70.974	36.802	1.00 0.00	В
35	MOTA	3693	CA	ILE	335	27.574	71.640	34.899	1.00 21.52	В
	ATOM	3694	CB	ILE	335	26.166	71.818	35.518	1.00 22.25	В
	ATOM	3695	CG2		335	26.288	72.266	36.946	1.00 30.01	B
	ATOM	3696		ILE	335	25.365	72.886	34.776	1.00 13.73	В
	ATOM	3697		ILE	335	25.018	72.533	33.362	1.00 25.02	В
40	ATOM	3698	C	ILE	335	28.053	72.976	34.345	1.00 24.47	B
10	ATOM	3699	Õ	ILE	335	28.012	73.203	33.135	1.00 23.62	В
	ATOM	3700	N	PHE	336	28.537	73.841	35.235	1.00 24.00	В
	ATOM	3701	H	PHE	336	28.593	73.575	36.176	1.00 24.00	В
	ATOM	3702	CA	PHE	336	28.987	75.179	34.848	1.00 29.92	В
45	ATOM	3703	CB	PHE	336	28.561	76.179	35.932	1.00 31.59	В
7.7	ATOM	3703	CG	PHE	336	27.077	76.412	35.973	1.00 26.05	В
	ATOM	3705		PHE	336	26.290	75.810	36.955	1.00 20.05	В
		3705		PHE	336	26.459	77.184	34.993	1.00 30.03	В
	ATOM						75.970	36.958	1.00 24.28	
50	MOTA	3707		PHE PHE	336	24.895		34.981	1.00 25.70	В
50	ATOM	3708			336	25.072	77.353			В
	MOTA	3709	CZ	PHE	336	24.287	76.738	35.971 34.495	1.00 22.17 1.00 31.44	В
	ATOM	3710	C	PHE	336	30.463	75.384		1.00 31.44	В
	ATOM	3711	0	PHE	336	30.870	76.491 74.328	34.124	1.00 27.91	В
55	MOTA	3712	N	ALA	337	31.260		34.583		В
55	ATOM	3713	H	ALA	337	30.895	73.465	34.875	1.00 0.00	В
	ATOM	3714	CA	ALA	337	32.674	74.440	34.253	1.00 35.57	В
	MOTA	3715	CB	ALA	337	33.518	74.124	35.479	1.00 31.23	В
	ATOM	3716	C	ALA	337	33.085	73.537	33.083	1.00 38.16	В
<b>CO</b>	MOTA	3717	0	ALA	337	33.755	73.989	32.162	1.00 40.82	В
60	MOTA	3718	N	LEU	338	32.668	72.271	33.125	1.00 41.05	В
	ATOM	3719	H	LEU	338	32.114	71.987	33.880	1.00 0.00	В
	ATOM	3720	CA	LEU	338	33.003	71.286	32.092	1.00 43.90	В
	ATOM	3721	CB	LEU	338	32.334	69.943	32.405	1.00 43.75	В
	ATOM	3722	CG	LEU	338	33.195	68.796	32.939	1.00 46.43	В
65	MOTA	3723		LEU	338	32.356	67.526	33.010	1.00 48.40	В
	MOTA	3724	CD2	LEU	338	34.406	68.586	32.043	1.00 46.34	В
	ATOM	3725	C	LEU	338	32.609	71.712	30.683	1.00 47.43	В
	MOTA	3726	0	LEU	338	33.390	71.430	29.740	1.00 47.18	В
	MOTA	3727	TO	LEU	338	31.518	72.308	30.541	1.00 50.73	В
70	ATOM	3728		H20	1	11.763	72.942	27.999	1.00 13.08	W
	ATOM	3729	H1	H20	1	12.196	72.994	27.149	1.00 0.00	W
	ATOM	3730	H2	H20	1	11.929	72.051	28.302	1.00 0.00	W
	ATOM	3731		H20	2	33.606	75.805	28.263	1.00 38.72	W

ATOM 3733 HI H20 2 33.652 75.559 29.186 1.00 0.00 W ATOM 3734 HI H20 2 33.674 76.762 28.267 1.00 0.00 W ATOM 3734 HI H20 2 3 36.774 76.783 -1.078 1.00 59.42 W ATOM 3735 HI H20 2 3 36.774 76.583 -1.078 1.00 59.00 W ATOM 3735 HI H20 3 46.762 77.129 -1.159 1.00 0.00 W ATOM 3736 HI H20 3 47.663 76.286 -0.894 1.00 0.00 W ATOM 3736 HI H20 4 17.892 53.996 32.166 1.00 12.25 W ATOM 3736 HI H20 4 17.892 53.996 32.166 1.00 12.25 W ATOM 3736 HI H20 4 17.892 53.996 32.166 1.00 12.25 W ATOM 3736 HI H20 4 17.892 53.996 32.166 1.00 12.25 W ATOM 3740 HI H20 5 27.946 56.312 24.504 1.00 0.00 W ATOM 3743 HI H20 6 32.852 77.437 33.359 1.00 0.00 W ATOM 3743 HI H20 6 32.852 77.437 33.359 1.00 0.00 W ATOM 3744 HI H20 6 32.852 77.437 33.359 1.00 0.00 W ATOM 3744 HI H20 6 32.852 77.437 33.359 1.00 0.00 W ATOM 3745 HI H20 6 32.852 77.437 33.359 1.00 0.00 W ATOM 3745 HI H20 6 32.852 77.437 33.359 1.00 0.00 W ATOM 3745 HI H20 6 32.852 77.437 33.359 1.00 0.00 W ATOM 3745 HI H20 6 32.852 77.437 33.359 1.00 0.00 W ATOM 3748 HI H20 7 7 16.940 51.246 HI H20 1.00 0.00 W ATOM 3748 HI H20 7 16.940 51.246 HI H20 1.00 0.00 W ATOM 3748 HI H20 8 33.359 1.00 0.00 W ATOM 3750 HI H20 8 33.359 1.00 0.00 W ATOM 3751 HI H20 8 33.359 1.00 0.00 W ATOM 3751 HI H20 8 33.359 1.00 0.00 W ATOM 3754 HI H20 8 33.359 1.00 0.00 W ATOM 3754 HI H20 8 33.359 1.00 0.00 W ATOM 3754 HI H20 8 33.359 1.00 0.00 W ATOM 3755 HI H20 8 33.359 1.00 0.00 W ATOM 3755 HI H20 8 33.359 1.00 0.00 W ATOM 3754 HI H20 8 33.359 1.00 0.00 W ATOM 3755 HI H20 8 33.359 1.00 0.00 W ATOM 3755 HI H20 8 13.148 PS 1.00 0.00 W ATOM 3755 HI H20 8 13.148 PS 1.00 0.00 W ATOM 3755 HI H20 10 37.012 G9.641 38.86 1.00 0.00 W ATOM 3755 HI H20 10 37.012 G9.641 38.86 1.00 0.00 W ATOM 3757 HI H20 10 37.012 G9.641 38.86 1.00 0.00 W ATOM 3757 HI H20 10 37.012 G9.641 38.86 1.00 0.00 W ATOM 3757 HI H20 10 37.012 G9.641 38.86 1.00 0.00 W ATOM 3758 HI H20 10 37.012 G9.641 38.86 1.00 0.00 W ATOM 3758 HI H20 10 37.012 G9.641 38.8										
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5 AROM 3736 H2 H20 3 47.662 76.280 -0.894 1.00 0.00 W AROM 3737 OH2 H20 4 17.892 53.996 3.2616 1.00 0.20.5 W AROM 3738 H1 H20 4 17.892 53.996 3.2616 1.00 0.20.5 W AROM 3739 H2 H20 4 17.561 53.146 2.907 1.00 0.00 W AROM 3740 OH2 H20 5 28.607 56.204 23.823 1.00 37.75 W AROM 3741 H1 H20 5 27.946 56.312 24.504 1.00 0.00 W AROM 3741 H1 H20 5 27.946 56.312 24.504 1.00 0.00 W AROM 3742 H2 H20 6 33.273 78.394 33.342 1.00 0.99.21 M AROM 3744 H1 H20 6 33.2852 77.437 33.345 1.00 0.90.0 W AROM 3744 H1 H20 6 32.852 77.437 33.345 1.00 0.00 W AROM 3744 H1 H20 6 32.852 77.437 33.345 1.00 0.00 W AROM 3744 H1 H20 6 32.852 77.437 33.359 1.00 0.00 W AROM 3744 H1 H20 6 32.852 77.437 33.359 1.00 0.00 W AROM 3744 H1 H20 6 32.852 77.437 33.359 1.00 0.00 W AROM 3744 H1 H20 6 32.852 77.437 33.359 1.00 0.00 W AROM 3744 H1 H20 8 13.870 78.571 16.889 1.00 42.50 W AROM 3744 H1 H20 8 13.870 78.571 16.889 1.00 40.00 W AROM 3744 H1 H20 8 13.870 78.571 13.844 1.00 15.88 W AROM 3751 H1 H20 8 13.870 78.571 13.844 1.00 15.88 W AROM 3751 H2 H20 9 25.865 90.956 -0.487 1.00 0.00 W AROM 3753 H1 H20 9 25.865 90.956 -0.487 1.00 0.00 W AROM 3755 OH2 H20 9 25.865 90.956 -0.487 1.00 0.146 W AROM 3755 OH2 H20 9 25.865 90.956 -0.487 1.00 0.00 W AROM 3755 OH2 H20 9 25.865 90.956 -0.487 1.00 0.00 W AROM 3755 H2 H20 10 37.018 69.613 37.294 1.00 0.00 W AROM 3755 H2 H20 10 37.018 69.613 37.294 1.00 0.00 W AROM 3755 H2 H20 10 37.18 69.613 37.294 1.00 0.00 W AROM 3755 H2 H20 10 37.18 69.613 37.294 1.00 0.00 W AROM 3755 H2 H20 10 37.218 69.613 37.294 1.00 0.00 W AROM 3755 H2 H20 11 24.707 79.474 26.157 1.00 0.00 W AROM 3756 H2 H20 11 24.707 79.474 26.157 1.00 0.00 W AROM 3756 H2 H20 11 24.707 79.474 26.157 1.00 0.00 W AROM 3758 H2 H20 11 24.928 79.255 27.628 1.00 0.00 W AROM 3766 H2 H20 11 24.928 79.255 27.628 1.00 0.00 W AROM 3768 H2 H20 11 24.928 79.255 27.628 1.00 0.00 W AROM 3768 H2 H20 11 24.928 79.255 27.628 1.00 0.00 W AROM 3768 H2 H20 12 18.858 90.364 4.00 10.00 W AROM 3768 H2 H20 12 18.458 90.938 90.374 1.00 0.00 W AROM 3768 H2 H20 12 19 40.839 90.337 1.00										M
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50       ATOM       3781       H2       H2O       18       15.258       41.449       43.107       1.00       0.00       W         ATOM       3782       OH2       H2O       19       40.329       91.816       -7.396       1.00       25.37       W         ATOM       3783       H1       H2O       19       39.913       91.345       -6.675       1.00       0.00       W         ATOM       3784       H2       H2O       19       40.631       92.636       -7.004       1.00       0.00       W         ATOM       3785       OH2       H2O       20       6.640       73.014       46.415       1.00       33.60       W         ATOM       3786       H1       H2O       20       6.989       73.098       45.531       1.00       0.00       W         ATOM       3789       H1       H2O       21       37.583       68.788       40.034       1.00       36.96       W         ATOM       3790       H2       H2O       21       37.026       69.000       39.287       1.00       0.00       W         ATOM       3791       OH2       H2O       22       5.										
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	MOTA	3805	H2 H2O	26	18.160	71.014	18.764	1.00 0.00	W
	MOTA	3806	ОН2 Н2О	27	12.412	74.571	-14.438	1.00 54.13	W
	MOTA	3807	н1 н20	27	11.645		-14.647	1.00 0.00	M
_	MOTA	3808	H2 H2O	27	12.947		-13.875	1.00 0.00	M
5	MOTA	3809	OH2 H2O	28	35.093	93.688	9.513	1.00 49.07	W
	ATOM	3810	H1 H2O	28	34.158	93.901	9.502	1.00 0.00	M
	MOTA ATOM	3811 3812	H2 H2O OH2 H2O	28 29	35.143 27.557	92.843 67.319	9.955 47.587	1.00 0.00 1.00 20.63	W W
	ATOM	3813	H1 H2O	29	28.387	67.684	47.271	1.00 20.03	W
10	ATOM	3814	H2 H2O	29	27.650	66.377	47.466	1.00 0.00	W
	ATOM	3815	OH2 H2O	30	12.145	50.693	37.668	1.00 22.09	M
	ATOM	3816	н1 н20	30	12.508	49.987	38.209	1.00 0.00	M
	ATOM	3817	H2 H2O	30	12.370	51.493	38.131	1.00 0.00	W
	ATOM	3818	он2 н2о	31	29.496	59.286	42.408	1.00 37.05	W
15	ATOM	3819	H1 H2O	31	30.012	59.213	43.211	1.00 0.00	W
	MOTA	3820	н2 н20	31	29.640	60.183	42.110	1.00 0.00	M
	ATOM	3821	он2 н2о	32	28.197	52.345	43.775	1.00 24.75	W
	MOTA	3822	H1 H2O	32	28.094	52.722	42.902	1.00 0.00	M
20	MOTA ATOM	3823 3824	H2 H2O OH2 H2O	32 33	28.541 23.054	51.469	43.622 -19.613	1.00 0.00 1.00 54.17	W W
20	ATOM	3825	H1 H2O	33	23.018		-20.264	1.00 0.00	W
	ATOM	3826	H2 H2O	33	23.144		-20.124	1.00 0.00	W
	ATOM	3827	OH2 H2O	34	11.508	89.358	-0.033	1.00 89.65	W
	MOTA	3828	H1 H2O	34	10.947	90.015	0.378	1.00 0.00	W
25	MOTA	3829	H2 H2O	34	11.860	88.850	0.697	1.00 0.00	W
	MOTA	3830	ОН2 Н2О	35	11.641	45.393	37.448	1.00 51.14	W
	MOTA	3831	H1 H2O	35	11.020	45.208	36.743	1.00 0.00	M
	ATOM	3832	H2 H2O	35	11.965	44.531	37.713	1.00 0.00	W
30	MOTA MOTA	3833 3834	OH2 H2O H1 H2O	36 36	20.569 20.797	40.000	37.790 37.007	1.00 29.17	W
50	ATOM	3835	H2 H2O	36	20.797	40.503 40.523	38.517	1.00 0.00 1.00 0.00	W W
	MOTA	3836	OH2 H2O	37	24.685	71.120	-9.820	1.00 43.88	M
	MOTA	3837	H1 H2O	37	25.328	70.841	-9.165	1.00 0.00	W
	ATOM	3838	H2 H2O	37	24.632		-10.426	1.00 0.00	W
35	MOTA	3839	OH2 H2O	38	17.308	85.319	37.723	1.00 34.44	W
	MOTA	3840	H1 H2O	38	18.044	85.879	37.954	1.00 0.00	M
	MOTA	3841	H2 H2O	38	17.596	84.434	37.953	1.00 0.00	M
	MOTA	3842	OH2 H2O	39	12.687	42.769	41.100	1.00 28.15	M
40	MOTA	3843	H1 H2O	39	12.510	41.844	40.940	1.00 0.00	W
40	MOTA MOTA	3844 3845	H2 H2O OH2 H2O	39 40	11.922 17.331	43.225 86.756	40.743 34.308	1.00 0.00 1.00 14.85	W W
	MOTA	3846	H1 H2O	40	18.021	87.306	34.677	1.00 14.83	W
	ATOM	3847	H2 H2O	40	17.772	85.936	34.083	1.00 0.00	W
	ATOM	3848	ОН2 Н2О	41	11.389	77.413	34.219	1.00 13.24	W
45	ATOM	3849	H1 H2O	41	11.834	76.632	33.886	1.00 0.00	W
	MOTA	3850	H2 H2O	41	11.955	77.724	34.927	1.00 0.00	W
	ATOM	3851	он2 н2о	42	22.064	47.418	49.189	1.00 21.90	W
	ATOM	3852	н1 н20	42	22.578	47.067	49.916	1.00 0.00	W
50	ATOM	3853	H2 H2O	42	21.955		49.399	1.00 0.00	W
30	ATOM ATOM	3854 3855	OH2 H2O H1 H2O	43 43	42.304 42.968	89.935 90.334	-4.829 -4.263	1.00 41.26 1.00 0.00	W W
	ATOM	3856	H2 H2O	43	41.497	90.399	-4.203	1.00 0.00	W
	ATOM	3857	OH2 H2O	44	20.332	50.701	49.638	1.00 34.52	W
	ATOM	3858	н1 н20	44	20.304	50.701	48.682	1.00 0.00	W
55	ATOM	3859	H2 H2O	44	20.709	51.553	49.866	1.00 0.00	W
	MOTA	3860	он2 н2о	45	29.753	79.163	20.128	1.00 29.41	W
	MOTA	3861	н1 н20	45	29.861	79.995	20.588	1.00 0.00	W
	MOTA	3862	н2 н20	45	30.517	78.646	20.388	1.00 0.00	W
60	ATOM	3863	он2 н2о	46	21.428	84.063	13.081	1.00 37.53	W
60	MOTA	3864	H1 H2O H2 H2O	46	21.980	83.848	12.332	1.00 0.00	W
	ATOM ATOM	3865 3866	H2 H2O OH2 H2O	46 47	$22.024 \\ 44.014$	84.033 87.180	13.833	1.00 0.00 1.00 42.34	W
	ATOM	3867	H1 H2O	47	44.816	87.537	0.493 0.112	1.00 42.34	W
	ATOM	3868	H2 H2O	47	44.255	86.949	1.390	1.00 0.00	W
65	ATOM	3869	OH2 H2O	48	10.349	58.686	20.367	1.00 54.51	W
	ATOM	3870	H1 H2O	48	11.088	58.206	20.745	1.00 0.00	W
	MOTA	3871	H2 H2O	48	10.744	59.467	19.982	1.00 0.00	W
	MOTA	3872	он2 н2о	50	23.990	56.220	51.509	1.00 25.41	W
~^	MOTA	3873	H1 H2O	50	23.268	55.601	51.628	1.00 0.00	W
70	ATOM	3874	н2 н20	50	24.178	56.195	50.573	1.00 0.00	W
	ATOM	3875	он2 н2о	51	14.872	75.264	-7.889	1.00 34.60	W
	ATOM	3876 3877	H1 H2O	51 51	15.737	75.461	-8.249	1.00 0.00	W
	ATOM	3877	н2 н20	51	15.004	75.262	-6.940	1.00 0.00	W

	ATOM	3878	ОН2 Н2О	52	29.495	53.936	48.249	1.00 35.09	W
	MOTA	3879	H1 H2O	52	30.382	53.691	48.511	1.00 0.00	W
	MOTA	3880	H2 H2O	52	28.980	53.881	49.050	1.00 0.00	W
	ATOM	3881	ОН2 Н2О	53	23.913	39.862	34.279	1.00 24.69	W
5	ATOM	3882	н1 н20	53	23.928	40.573	34.917	1.00 0.00	W
	MOTA	3883	н2 н20	53	22.981	39.718	34.101	1.00 0.00	M
	MOTA	3884	он2 н20	54	27.855	38.735	36.184	1.00 41.97	W
	ATOM	3885	H1 H2O	54	27.501	37.874	35.965	1.00 0.00	W
10	MOTA	3886	H2 H2O	54	27.094	39.319	36.159	1.00 0.00	W
10	ATOM	3887	OH2 H2O	55	14.443	71.878	19.001 18.533	1.00 43.17 1.00 0.00	W
	ATOM	3888 3889	H1 H2O H2 H2O	55 55	13.698 14.053	71.493 72.271	19.782	1.00 0.00	M
	MOTA ATOM	3890	OH2 H2O	56	9.281	50.087	37.191	1.00 22.03	M
	ATOM	3891	H1 H2O	56	10.124	49.922	36.769	1.00 0.00	W
15	ATOM	3892	H2 H2O	56	9.351	49.660	38.045	1.00 0.00	W
	ATOM	3893	OH2 H2O	57	22.892	77.131	20.524	1.00 38.72	W
	ATOM	3894	н1 н20	57	22.303	76.460	20.869	1.00 0.00	W
	ATOM	3895	H2 H2O	57	22.962	76.933	19.591	1.00 0.00	W
	MOTA	3896	он2 н20	58	38.306	78.270	13.963	1.00 28.31	W
20	MOTA	3897	H1 H2O	58	38.886	77.518	14.102	1.00 0.00	M
	MOTA	3898	H2 H2O	58	37.541	77.899	13.520	1.00 0.00	W
	MOTA	3899	он2 н2о	59	10.937	66.046	49.581	1.00 34.62	W
	MOTA	3900	н1 н20	59	11.082	66.814	49.032	1.00 0.00	W
25	ATOM	3901	H2 H2O	59	11.613 40.917	65.426	49.320 -4.294	1.00 0.00 1.00 39.29	W W
25	MOTA	3902 3903	OH2 H2O H1 H2O	60 60	40.917	80.629 81.265	-5.010	1.00 39.29	W
	ATOM ATOM	3903	H2 H2O	60	41.832	80.403	-4.141	1.00 0.00	W
	ATOM	3905	OH2 H2O	61	37.462	76.032	26.379	1.00 35.75	W
	MOTA	3906	H1 H2O	61	37.318	75.396	27.075	1.00 0.00	W
30	MOTA	3907	H2 H2O	61	36.637	76.059	25.897	1.00 0.00	M
	ATOM	3908	OH2 H2O	62	12.194	92.917	7.443	1.00 26.35	M
	MOTA	3909	H1 H2O	62	12.299	93.860	7.569	1.00 0.00	W
	MOTA	3910	H2 H2O	62	12.553	92.749	6.576	1.00 0.00	M
2.5	ATOM	3911	ОН2 Н2О	63	10.746	48.472	38.472	1.00 32.24	W
35	ATOM	3912	H1 H2O	63	11.037	49.361	38.660	1.00 0.00	W
	ATOM	3913	H2 H2O	63	11.406	47.907 73.773	38.868 41.569	1.00 0.00 1.00 29.16	W W
	ATOM ATOM	391 <b>4</b> 3915	ОН2 Н2О Н1 Н2О	64 64	24.609 24.846	74.155	42.417	1.00 23.10	W
	ATOM	3916	H2 H2O	64	25.433	73.754	41.081	1.00 0.00	W
40	ATOM	3917	OH2 H2O	65	30.012	66.185	-8.084	1.00 59.17	W
	ATOM	3918	H1 H2O	65	30.800	66.596	-7.731	1.00 0.00	W
	ATOM	3919	H2 H2O	65	29.658	66.832	-8.697	1.00 0.00	M
	MOTA	3920	OH2 H2O	66	31.620	57.288	44.605	1.00 33.39	M
	ATOM	3921	H1 H2O	66	30.791	56.867	44.837	1.00 0.00	M
45	ATOM	3922	H2 H2O	66	31.532	57.494	43.676	1.00 0.00	W
	MOTA	3923	он2 н20	67	18.628	82.133	47.615 47.779	1.00 41.34	W
	MOTA	3924 3925	H1 H2O H2 H2O	67 67	19.144 18.596	81.345 82.582	48.458	1.00 0.00	W
	ATOM ATOM	3926	OH2 H2O	68	26.118		16.428	1.00 16.27	W
50	MOTA	3927	H1 H2O	68	25.731	86.540	17.305	1.00 0.00	W
50	MOTA	3928	H2 H2O	68	26.764	87.261	16.467	1.00 0.00	W
	ATOM	3929	OH2 H2O	69	6.149	45.998	26.772	1.00 58.89	W
	MOTA	3930	H1 H2O	69	6.523	46.223	27.625	1.00 0.00	W
	MOTA	3931	H2 H2O	69	5.200	46.037	26.914	1.00 0.00	W
55	MOTA	3932	он2 н2о	70	7.387	86.734	36.372	1.00 26.69	W
	MOTA	3933	H1 H2O	70	7.690	87.232	35.613	1.00 0.00	W
	MOTA	3934	H2 H2O	70	6.557	87.153	36.615	1.00 0.00 1.00 20.12	W
	MOTA	3935 3936	OH2 H2O	71 71	19.016 19.744	50.608 51.094	41.020 41.405	1.00 20.12	W W
60	MOTA MOTA	3937	H1 H2O H2 H2O	71	18.765	51.119	40.254	1.00 0.00	W
00	ATOM	3938	OH2 H2O	72	22.966	54.069	53.338	1.00 58.44	W
	ATOM	3939	H1 H2O	72	22.736	53.762	54.218	1.00 0.00	W
	ATOM	3940	H2 H2O	72	23.801	54.525	53.458	1.00 0.00	W
	ATOM	3941	ОН2 Н2О	73	32.935	84.107	34.520	1.00 38.39	W
65	ATOM	3942	H1 H2O	73	32.932	85.062	34.520	1.00 0.00	W
	ATOM	3943	H2 H2O	73	32.932	83.865	33.593	1.00 0.00	W
	ATOM	3944	ОН2 Н2О	74	15.144	50.152	34.763	1.00 15.36	M
	MOTA	3945	н1 н20	74	15.994	49.728	34.642	1.00 0.00	W
70	ATOM	3946	H2 H2O	74	14.963	50.062	35.700	1.00 0.00	W
70	ATOM	3947	OH2 H2O	75 75	39.834 39.093	73.517 73.212	37.279 37.805	1.00 21.08 1.00 0.00	W W
	ATOM	3948 3949	H1 H2O H2 H2O	75 75	39.093	74.465	37.805	1.00 0.00	W
	ATOM ATOM	3950	OH2 H2O	75 76	5.621	49.847	47.235	1.00 36.63	W
	ALON	5,500	J.12 112 J	. 5	5.041	15.04/	1		••

	MOTA	3951	H1 H2O	76	5.682	50.181	48.127	1.00 0.00	W
	MOTA	3952	H2 H2O	76	6.291	50.328	46.749	1.00 0.00	W
	MOTA	3953	ОН2 Н2О	77	20.855	42.150	47.963	1.00 45.89	W
~	MOTA	3954	H1 H2O	77	21.782	42.249	47.739	1.00 0.00	W
5	ATOM	3955	H2 H2O	77	20.797 8.330	41.284	48.366	1.00 0.00	W
	ATOM ATOM	3956 3957	ОН2 Н2О Н1 Н2О	78 78	8.581	65.636 66.186	18.869 18.125	1.00 38.49 1.00 0.00	W W
	ATOM	3958	H2 H2O	78	8.184	66.254	19.584	1.00 0.00	W
	ATOM	3959	OH2 H2O	79	37.225	73.080	47.421	1.00 42.94	W
10	ATOM	3960	H1 H2O	79	37.775	72.667	46.755	1.00 0.00	W
	ATOM	3961	H2 H2O	79	36.353	73.108	47.030	1.00 0.00	W
	MOTA	3962	OH2 H2O	80	36.019	65.979	41.953	1.00 34.15	W
	MOTA	3963	H1 H2O	80	36.913	65.996	42.303	1.00 0.00	M
1.5	ATOM	3964	H2 H2O	80	35.821	65.048	41.856	1.00 0.00	W
15	MOTA	3965	OH2 H2O	81	37.936	72.735	-2.902	1.00 58.65	W
	MOTA MOTA	3966 3967	H1 H2O H2 H2O	81 81	38.631 37.913	73.117 73.277	-2.367 -3.690	1.00 0.00 1.00 0.00	W
	ATOM	3968	OH2 H2O	82	23.143	50.854	55.229	1.00 73.08	W W
	MOTA	3969	H1 H2O	82	22.200	50.699	55.185	1.00 0.00	W
20	MOTA	3970	H2 H2O	82	23.429	50.377	56.008	1.00 0.00	W
	MOTA	3971	OH2 H2O	83	35.270	96.894	-8.992	1.00 46.37	W
	MOTA	3972	H1 H2O	83	34.385	97.082	-9.298	1.00 0.00	W
	MOTA	3973	H2 H2O	83	35.800	97.621	-9.320	1.00 0.00	W
25	MOTA MOTA	3974 3975	OH2 H2O	84	34.683 35.001	68.046	40.254	1.00 41.87	W
45	ATOM	3976	H1 H2O H2 H2O	84 84	33.743	67.185 68.022	39.981 40.069	1.00 0.00 1.00 0.00	W
	ATOM	3977	OH2 H2O	85	7.937	93.884	8.479	1.00 67.26	W W
	MOTA	3978	H1 H2O	85	8.505	93.128	8.331	1.00 0.00	W
	ATOM	3979	H2 H2O	85	7.793	94.250	7.607	1.00 0.00	W
30	MOTA	3980	ОН2 Н2О	86	41.437	88.270	5.694	1.00 43.07	W
	ATOM	3981	н1 н20	86	40.650	88.680	6.057	1.00 0.00	W
	ATOM	3982	H2 H2O	86	41.183	87.355	5.556	1.00 0.00	W
	ATOM ATOM	3983 3984	он2 н2о н1 н2о	87 87	18.418 19.346	89.968 89.974	41.295	1.00 50.98	W
35	ATOM	3985	H2 H2O	87	18.287	89.127	41.525 40.854	1.00 0.00 1.00 0.00	W W
30	ATOM	3986	OH2 H2O	88	15.346	97.033	5.772	1.00 51.64	W
	ATOM	3987	H1 H2O	88	14.535	97.052	5.262	1.00 0.00	W
	ATOM	3988	H2 H2O	88	15.780	96.224	5.502	1.00 0.00	W
40	ATOM	3989	он2 н2о	89	47.753	89.370	-3.781	1.00 37.41	W
40	ATOM	3990	H1 H2O	89	47.756	90.330	-3.781	1.00 0.00	W
	MOTA MOTA	3991 3992	H2 H2O OH2 H2O	89 90	47.756 17.822	89.133 70.217	-4.708	1.00 0.00	W
	ATOM	3993	H1 H2O	90	18.493	70.890	21.038 21.166	1.00 53.57 1.00 0.00	W W
	ATOM	3994	H2 H2O	90	17.151	70.426	21.692	1.00 0.00	W
45	MOTA	3995	OH2 H2O	91	2.696	51.590	41.944	1.00 46.78	W
	MOTA	3996	н1 н20	91	1.893	51.743	42.439	1.00 0.00	W
	ATOM	3997	н2 н20	91	3.400	51.837	42.544	1.00 0.00	W
	ATOM	3998	OH2 H2O	95	34.676	75.860	41.073	1.00 39.50	W
50	ATOM ATOM	3999 4000	H1 H2O H2 H2O	95 95	35.228	75.793		1.00 0.00	W
30	ATOM	4000	OH2 H2O	96	34.453 39.675	74.957 76.625	41.286 -9.371	1.00 0.00 1.00 56.41	W
	ATOM	4002	H1 H2O	96	38.896	76.095	-9.211	1.00 0.00	W
	ATOM	4003	H2 H2O	96	40.385	75.984	-9.456	1.00 0.00	W
	ATOM	4004	он2 н2о	97	18.254	64.042	7.803	1.00 55.42	W
55	ATOM	4005	н1 н20	97	18.067	64.981	7.768	1.00 0.00	W
	ATOM	4006	H2 H2O	97	17.406	63.636	7.982	1.00 0.00	W
	MOTA MOTA	4007 4008	ОН2 Н2О Н1 Н2О	99	36.040 35.612	76.842	46.828	1.00 41.76	W
	ATOM	4009	H2 H2O	99 99	35.367	76.180 77.514	46.290 46.962	1.00 0.00	W
60	ATOM	4010	OH2 H2O	100	39.087		-12.653	1.00 50.93	W
-	ATOM	4011	H1 H2O	100	39.148		-13.482	1.00 0.00	M
	ATOM	4012	H2 H2O	100	39.394	91.370	-11.997	1.00 0.00	W
	ATOM	4013	он2 н2о	102	34.315	73.486	18.013	1.00 32.56	W
<i>(</i> =	MOTA	4014	н1 н20	102	34.941	73.597	17.299	1.00 0.00	M
65	MOTA	4015	H2 H2O	102	33.483	73.303	17.577	1.00 0.00	W
	ATOM ATOM	4016 4017	ОН2 Н2О Н1 Н2О	103 103	27.629	65.918	7.501 8.130	1.00 26.86	W
	ATOM	4017	H1 H2O H2 H2O	103	26.981 28.387	65.607 65.342	7.634	1.00 0.00 1.00 0.00	W
	ATOM	4019	OH2 H2O	104	30.549		-10.939	1.00 52.39	W
70	ATOM	4020	H1 H2O	104	30.082		-11.415	1.00 0.00	W
	ATOM	4021	н2 н20	104	30.530		-11.524	1.00 0.00	W
	MOTA	4022	он2 н2о	105	34.538	71.979	38.560	1.00 30.69	W
	MOTA	4023	н1 н20	105	33.720	72.302	38.185	1.00 0.00	W

	ATOM	4024	H2 H2	0 105	34.317	71.734	39.455	1.00 0.00	W
	ATOM	4025	OH2 H2	0 106	31.168	67.923	13.585	1.00 47.02	W
	MOTA	4026	H1 H2		31.193	67.876	14.540	1.00 0.00	W
	MOTA	4027	H2 H2	0 106	30.514	68.599	13.396	1.00 0.00	W
5	MOTA	4028	OH2 H2	0 107		63.732	44.548	1.00 33.54	W
	ATOM	4029	H1 H2	0 107	32.546	63.550	45.458	1.00 0.00	W
	ATOM	4030	H2 H2	0 107	33.687	63.411	44.472	1.00 0.00	W
	ATOM	4031	он2 н2	0 108	19.475	88.576	35.346	1.00 35.25	W
	MOTA	4032	H1 H2	0 108	19.617	88.129	34.508	1.00 0.00	W
10	MOTA	4033	H2 H2			88.319	35.881	1.00 0.00	W
	MOTA	4034	он2 н2			52.354	23.080	1.00 48.58	W
	MOTA	4035	H1 H2			52.051	22.499	1.00 0.00	W
	MOTA	4036	H2 H2			52.922	23.711	1.00 0.00	W
. ~	MOTA	4037	OH2 H2			52.640	32.308	1.00 51.66	W
15	ATOM	4038	H1 H2			52.563	31.371	1.00 0.00	W
	ATOM	4039	H2 H2			52.644	32.711	1.00 0.00	W
	ATOM	4040	OH2 H2			60.681	13.605	1.00 55.65	W
	ATOM	4041	H1 H2			60.785	12.718	1.00 0.00	W
20	MOTA	4042	H2 H2			61.054	13.557	1.00 0.00	W
20	MOTA	4043	OH2 H2		38.699	63.142	37.584	1.00 49.09	W
	ATOM	4044	H1 H2			62.845	37.265	1.00 0.00	W
	ATOM ATOM	4045 4046	H2 H2 OH2 H2		39.233	62.347	37.604	1.00 0.00	W
	ATOM	4046			31.344 31.126	57.427 56.895	39.398	1.00 37.73	W
25	ATOM	4047	H1 H2 H2 H2			57.933	40.166	1.00 0.00	W
25	ATOM	4048	OH2 H2		41.350	83.449	39.226 -8.714	1.00 0.00 1.00 60.04	W
	ATOM	4050	H1 H2			83.752	-9.569	1.00 0.04	W
	ATOM	4051	H2 H2		41.043	84.130	-8.103	1.00 0.00	W W
	ATOM	4052	OH2 H2		42.987	90.912	5.698	1.00 0.00	W
30	ATOM	4053	H1 H2		42.742	89.993	5.572	1.00 30.99	W
30	ATOM	4054	H2 H2			90.888	5.853	1.00 0.00	W
	ATOM	4055	OH2 H2			71.465	53.783	1.00 33.44	W
	MOTA	4056	H1 H2			72.422	53.780	1.00 0.00	W
	ATOM	4057	H2 H2		27.239	71.225	52.853	1.00 0.00	W
35	ATOM	4058	OH2 H2		11.225	50.304	22.316	1.00 55.33	W
	ATOM	4059	H1 H2		11.185	51.196	22.657	1.00 0.00	W
	ATOM	4060	H2 H2			50.343	21.483	1.00 0.00	W
	MOTA	4061	он2 н2		10.516	74.345	13.709	1.00 49.01	W
	MOTA	4062	н1 н2	0 122	11.305	74.880	13.770	1.00 0.00	W
40	MOTA	4063	H2 H2		10.747	73.529	14.153	1.00 0.00	W
	MOTA	4064	ОН2 Н2	0 123	21.221	81.929	43.450	1.00 35.78	W
	MOTA	4065	н1 н2	0 123	20.410	82.390	43.227	1.00 0.00	W
	MOTA	4066	H2 H2	0 123	21.623	82.469	44.129	1.00 0.00	W
	ATOM	4067	он2 н2		26.901	87.147	37.889	1.00 67.29	W
45	MOTA	4068	H1 H2			87.057	37.631	1.00 0.00	W
	ATOM	4069	H2 H2			86.709	38.739	1.00 0.00	W
	MOTA	4070	OH2 H2			73.517	7.577	1.00 47.94	M
	ATOM	4071	H1 H2		38.835	73.559	7.101	1.00 0.00	W
<b>50</b>	ATOM	4072	H2 H2			73.253		1.00 0.00	W
50	ATOM	4073	он2 н2			70.971	29.298	1.00 20.65	W
	MOTA	4074	H1 H2					1.00 0.00	W
	ATOM	4075	H2 H2			71.385	30.132	1.00 0.00	M
	MOTA	4076	OH2 H2			81.404	36.223	1.00 27.14	M
55	MOTA	4077	H1 H2			81.595 81.776	36.500	1.00 0.00	M
33	ATOM	4078	H2 H2 OH2 H2		6.195 13.263		36.918	1.00 0.00	W
	ATOM ATOM	4079			13.263	68.119	49.513	1.00 44.60	W
	ATOM	4080 4081	H1 H2 H2 H2			67.240	49.144	1.00 0.00	W
	ATOM	4082	OH2 H2		13.500 19.524	68.707	48.799 -11.380	1.00 0.00 1.00 25.22	W W
60	ATOM	4083	H1 H2				-11.380 $-10.742$	1.00 23.22	W
00	ATOM	4084	H2 H2				-11.875	1.00 0.00	W
	ATOM	4085	OH2 H2		40.212	59.845	25.750	1.00 51.43	W
	MOTA	4086	H1 H2		41.124		26.015	1.00 0.00	W
	ATOM	4087	H2 H2		40.235	59.869	24.793	1.00 0.00	W
65	ATOM	4088	OH2 H2			100.636	-9.493	1.00 47.67	W
0.5	ATOM	4089	H1 H2			100.030	-9.422	1.00 47.67	W
	ATOM	4090	H2 H2			101.276	-9.363	1.00 0.00	W
	ATOM	4091	OH2 H2			75.485	18.573	1.00 47.00	W
	ATOM	4092	H1 H2			76.396	18.784	1.00 47.00	W
70	ATOM	4093	H2 H2		6.759	75.513	18.008	1.00 0.00	W
	ATOM	4094	он2 н2		25.465	59.184	52.290	1.00 28.76	W
	ATOM	4095	H1 H2		25.749		51.420	1.00 0.00	W
	ATOM	4096	H2 H2		24.512	59.318	52.281	1.00 0.00	W

	ATOM	4097	ОН2 Н2О	140	14.960	69.189	7.890	1.00 46.58	W
	MOTA	4098	н1 н20	140	14.139	69.668	7.972	1.00 0.00	W
	ATOM	4099	H2 H2O	140	15.631	69.867	7.811	1.00 0.00	W
	MOTA	4100	OH2 H2O	142	31.562	73.845	26.725	1.00 46.85	W
5	MOTA	4101	H1 H2O	142	30.757	74.357	26.741	1.00 0.00	W
	ATOM	4102	H2 H2O	142	31.916	73.978	25.843	1.00 0.00	W
	ATOM	4103	он2 н2о	143	24.525	81.714	35.572	1.00 45.84	W
	ATOM	4104	H1 H2O	143	23.681	81.414	35.237	1.00 0.00	W
	ATOM	4105	H2 H2O	143	25.142	81.535	34.862	1.00 0.00	W
10	ATOM	4106	ОН2 Н2О	144	30.404	37.547	38.155	1.00 49.49	W
	ATOM	4107	H1 H2O	144	31.040	37.919	38.772	1.00 0.00	W
	ATOM	4108	H2 H2O	144	29.868	38.295	37.890	1.00 0.00	W
	ATOM	4109	ОН2 Н2О	145	18.510	37.954	48.005	1.00 31.26	W
	ATOM	4110	H1 H2O	145	18.573	37.366	48.753	1.00 0.00	W
15	ATOM	4111	H2 H2O	145	19.251	37.719	47.448	1.00 0.00	W
	MOTA	4112	OH2 H2O	148			-11.072	1.00 69.13	W
	ATOM	4113	H1 H2O	148			-10.238	1.00 0.00	W
	MOTA	4114	H2 H2O	148			-11.127	1.00 0.00	W
	MOTA	4115	OH2 H2O	149	30.616	69.892	11.062	1.00 59.13	W
20	MOTA	4116	н1 н20	149	30.597	69.088	10.544	1.00 0.00	W
	ATOM	4117	H2 H2O	149	31.534	69.990	11.317	1.00 0.00	W
	ATOM	4118	OH2 H2O	151	22.397		-18.890	1.00 49.14	W
	ATOM	4119	н1 н20	151	22.660		-19.796	1.00 0.00	W
	ATOM	4120	H2 H2O	151	22.588		-18.750	1.00 0.00	W
25	ATOM	4121	ОН2 Н2О	152	23.997	68.719	-3.081	1.00 37.05	W
	ATOM	4122	H1 H2O	152	23.944	69.622	-3.393	1.00 0.00	W
	ATOM	4123	H2 H2O	152	23.498	68.717	-2.264	1.00 0.00	W
	MOTA	4124	ОН2 Н2О	153	6.761	78.049	41.002	1.00 44.92	W
	MOTA	4125	H1 H2O	153	6.495	77.572	40.213	1.00 0.00	w
30	ATOM	4126	H2 H2O	153	7.695	77.879	41.080	1.00 0.00	W
	ATOM	4127	он2 н2о	154	14.604	84.085	47.918	1.00 27.17	W
	MOTA	4128	н1 н20	154	14.800	83.921	48.839	1.00 0.00	W
	MOTA	4129	H2 H2O	154	15.458	84.196	47.504	1.00 0.00	W
	MOTA	4130	ОН2 Н2О	157	20.208	87.608	38.773	1.00 46.36	W
35	ATOM	4131	H1 H2O	157	19.447	88.077	38.424	1.00 0.00	M
	MOTA	4132	H2 H2O	157	20.838	88.299	38.980	1.00 0.00	W
	ATOM	4133	OH2 H2O	161	27.786	81.756	30.433	1.00 20.04	W
	ATOM	4134	H1 H2O	161	27.657	81.992	31.345	1.00 0.00	W
	MOTA	4135	H2 H2O	161	27.013	81.230	30.207	1.00 0.00	W
40	ATOM	4136	OH2 H2O	162	25.545	41.107	41.204	1.00 39.67	W
	ATOM	4137	H1 H2O	162	26.123	40.371	41.410	1.00 0.00	W
	MOTA	4138	H2 H2O	162	24.668	40.789	41.410	1.00 0.00	W
	ATOM	4139	OH2 H2O	163	34.968	61.130	39.718	1.00 58.53	W
	MOTA	4140	н1 н20	163	35.625	61.220	40.410	1.00 0.00	W
45	MOTA	4141	H2 H2O	163	34.194	60.792	40.166	1.00 0.00	W
	MOTA	4142	он2 н2о	164	31.867	61.174	40.931	1.00 30.31	W
	ATOM	4143	н1 н20	164	31.027	60.812	40.654	1.00 0.00	W
	ATOM	4144	H2 H2O	164	31.803	61.239	41.882	1.00 0.00	W
<b>70</b>	ATOM	4145	он2 н2о	165	18.529	51.777	47.785	1.00 26.36	W
50	ATOM	4146	H1 H2O	165	18.240	52.561	48.263	1.00 0.00	M
	ATOM	4147	H2 H2O	165	18.619	51.109	48.456	1.00 0.00	W
	ATOM	4148	OH2 H2O	166	6.824	56.798	46.694	1.00 31.23	W
	ATOM	4149	H1 H2O	166	7.339	56.878	47.493	1.00 0.00	W
<i>E E</i>	ATOM	4150	H2 H2O	166	5.921	56.982	46.973	1.00 0.00	W
55	ATOM	4151	OH2 H2O	167	4.124	74.966	21.486	1.00 35.69	W
	ATOM	4152	H1 H2O	167	4.300	75.262	20.590	1.00 0.00	W
	ATOM	4153	H2 H2O	167	4.736	75.467	22.026	1.00 0.00	W
	ATOM	4154	ОН2 Н2О	168	23.115		-19.644	1.00 56.66	M
60	ATOM	4155	н1 н20	168	23.431		-20.521	1.00 0.00	W
00	ATOM	4156	H2 H2O	168	23.194		-19.152	1.00 0.00	W
	ATOM	4157	OH2 H2O	169	3.381	70.239	27.505	1.00 32.76	M
	ATOM	4158	H1 H2O	169	2.709	70.126	26.830	1.00 0.00	W
	ATOM	4159	H2 H2O	169	3.950	70.929	27.161	1.00 0.00	W
65	ATOM	4160	OH2 H2O	170	38.354	96.654	-4.019	1.00 38.96	W
UJ	ATOM	4161	H1 H2O	170	38.897	97.181	-4.602	1.00 0.00	M
	ATOM	4162	H2 H2O	170	38.910	95.925	-3.757	1.00 0.00	W
	ATOM	4163	OH2 H2O	$\frac{171}{171}$	31.765	75.253	24.200	1.00 35.79	W
	ATOM	4164	H1 H2O	171	31.801	76.033	23.651	1.00 0.00	W
70	ATOM	4165 4166	H2 H2O	171	32.622	74.840	24.093	1.00 0.00	W
70	ATOM ATOM	4166	ОН2 Н2О Н1 Н2О	172 172	30.112 29.550	51.159	46.701	1.00 42.99	W
	ATOM	4168	H2 H2O	172	30.504	51.828	47.094	1.00 0.00	W
	ATOM	4169	OH2 H2O	173	14.724	50.708 60.204	47.449 $54.146$	1.00 0.00	W
	AL OH	エエリブ	V112 112U	113	14./44	00.204	74.T40	1.00 44.12	W

	ATOM	4170	H1 H2O	173	13.852	60.500	54.408	1.00 0.00	W
	MOTA	4171	H2 H2O	173	15.149	59.955	54.966	1.00 0.00	W
	ATOM	4172	он2 н2о	174	34.426	92.105	20.174	1.00 43.09	W
	ATOM	4173	H1 H2O	174	33.995	92.193	19.323	1.00 0.00	W
5	MOTA	4174	H2 H2O	174	35.110	92.775	20.165	1.00 0.00	W
	ATOM	4175	OH2 H2O	175	15.079	77.472	19.106	1.00 26.05	W
	ATOM	4176	Н1 Н2О	175	15.197	78.034	19.868	1.00 0.00	W
	MOTA	4177	H2 H2O	175	14.807	76.627	19.465	1.00 0.00	W
	ATOM	4178	OH2 H2O	176	4.428	65.813	39.483	1.00 41.04	W
10	ATOM	4179	н1 н20	176	4.482	66.597	38.935	1.00 0.00	W
	MOTA	4180	H2 H2O	176	3.948	66.099	40.261	1.00 0.00	W
	ATOM	4181	ОН2 Н2О	177	15.709	70.351	-5.398	1.00 60.42	W
	MOTA	4182	н1 н20	177	15.048	70.541	-4.731	1.00 0.00	W
	ATOM	4183	H2 H2O	177	15.488	69.475	-5.712	1.00 0.00	W
15	ATOM	4184	ОН2 Н2О	178	33.370	76.092	46.298	1.00 73.91	W
	ATOM	4185	н1 н20	178	32.527	75.849	46.680	1.00 0.00	W
	ATOM	4186	H2 H2O	178	33.647	76.862	46.791	1.00 0.00	W
	ATOM	4187	ОН2 Н2О	179	32.160	88.256	-3.330	1.00 31.03	W
	ATOM	4188	H1 H2O	179	31.330	88.041	-3.759	1.00 0.00	W
20	ATOM	4189	H2 H2O	179	32.571	88.893	-3.916	1.00 0.00	W
	ATOM	4190	он2 н2о	180	43.785	91.145	1.609	1.00 42.82	W
	MOTA	4191	H1 H2O	180	44.441	91.779	1.325	1.00 0.00	W
	MOTA	4192	H2 H2O	180	44.208	90.654	2.311	1.00 0.00	W
	MOTA	4193	OH2 H2O	181	23.220	65.998	2.718	1.00 25.59	W
25	ATOM	4194	H1 H2O	181	22.845	66.784	2.330	1.00 0.00	W
	MOTA	4195	H2 H2O	181	22.846	65.275	2.212	1.00 0.00	W
	MOTA	4196	OH2 H2O	182	7.003	43.420	24.621	1.00 50.96	W
	ATOM	4197	H1 H2O	182	7.061	43.954	25.414	1.00 0.00	W
••	ATOM	4198	H2 H2O	182	7.912	43.254	24.376	1.00 0.00	M
30	MOTA	4199	ОН2 Н2О	183	27.129	44.901	42.342	1.00 61.07	W
	MOTA	4200	н1 н20	183	26.349	45.392	42.607	1.00 0.00	W
	MOTA	4201	H2 H2O	183	27.383	44.415	43.126	1.00 0.00	W
	ATOM	4202	ОН2 Н2О	184	20.120	62.615	6.341	1.00 52.42	W
25	ATOM	4203	H1 H2O	184	19.717	63.462	6.535	1.00 0.00	W
35	ATOM	4204	H2 H2O	184	20.224	62.197	7.197	1.00 0.00	W
	ATOM	4205	OH2 H2O	186	10.038	94.189	-8.999	1.00 40.69	W
	ATOM	4206 4207	H1 H2O H2 H2O	186	10.000	93.361	-9.481	1.00 0.00	W
	ATOM ATOM	4207	H2 H2O OH2 H2O	186 187	9.190 39.048	94.600	-9.161	1.00 0.00	W
40	ATOM	4209	H1 H2O	187	39.048	78.109 79.067	48.627 48.627	1.00 43.94 1.00 0.00	W
10	ATOM	4210	H2 H2O	187	39.049	77.870	47.700	1.00 0.00	W
	MOTA	4211	OH2 H2O	188	29.997	88.546	37.175	1.00 66.02	W
	ATOM	4212	H1 H2O	188	29.998	89.503	37.176	1.00 00.02	M
	ATOM	4213	H2 H2O	188	29.998	88.306	36.249	1.00 0.00	W
45	ATOM	4214	OH2 H2O	189	33.213	66.563	16.332	1.00 62.88	W
	ATOM	4215	H1 H2O	189	33.911	66.201	15.788	1.00 0.00	W
	MOTA	4216	н2 н20	189	33.092	67.455	16.008	1.00 0.00	W
	ATOM	4217	OH2 H2O	190	29.894	60.575	22.671	1.00 41.27	W
	MOTA	4218	H1 H2O	190	29.363	61.361	22.549	1.00 0.00	W
50	ATOM	4219	H2 H2O	190	30.767	60.909	22.889	1.00 0.00	W
	ATOM	4220	OH2 H2O	191	17.276	53.069	43.250	1.00 10.66	W
	MOTA	4221	н1 н20	191	17.592	53.312	44.119	1.00 0.00	W
	ATOM	4222	H2 H2O	191	18.045	52.689	42.817	1.00 0.00	W
	ATOM	4223	он2 н2о	192	35.647	59.655	27.750	1.00 26.14	W
55	ATOM	4224	H1 H2O	192	36.404	59.816	28.311	1.00 0.00	W
	ATOM	4225	H2 H2O	192	35.899	60.010	26.897	1.00 0.00	W
	ATOM	4226	он2 н2о	193	38.775	60.787	30.053	1.00 36.89	M
	ATOM	4227	н1 н20	193	38.108	61.130	29.455	1.00 0.00	W
<b>(0</b>	ATOM	4228	H2 H2O	193	39.557	61.302	29.857	1.00 0.00	W
60	MOTA	4229	он2 н2о	194	18.790	80.718	52.778	1.00 28.10	M
	ATOM	4230	н1 н20	194	18.791	81.672	52.780	1.00 0.00	W
	ATOM	4231	H2 H2O	194	18.791	80.475	51.853	1.00 0.00	M
	ATOM	4232	он2 н20	195	22.571	68.265	53.229	1.00 34.42	W
65	ATOM	4233	H1 H2O	195	23.152	67.936	53.916	1.00 0.00	M
65	MOTA	4234	H2 H2O	195	22.266	69.110	53.558	1.00 0.00	W
	ATOM	4235	OH2 H2O	196	7.904	98.993	-8.160	1.00 39.75	W
	ATOM	4236	H1 H2O	196	7.904	99.952	-8.160	1.00 0.00	W
	ATOM	4237	H2 H2O	196	7.904	98.755	-9.087	1.00 0.00	W
70	ATOM	4238	OH2 H2O	197	15.117	76.593	49.958	1.00 44.24	W
10	MOTA	4239 4240	H1 H2O H2 H2O	197 197	14.700 15.264	76.989	50.724	1.00 0.00	W
	ATOM ATOM	4240	H2 H2O OH2 H2O	197	18.738	77.325 61.062	49.360	1.00 0.00	W Ta7
	MOTA	4241	H1 H2O	198	18.739	62.019	5.012 5.011	1.00 57.29 1.00 0.00	W
	111 011	-~ <del></del>	1120	170	10.733	02.017	2.011	1.00 0.00	VV

	Z TPOM	1212	H3 H30	100	10 720	60 000	1 004	1 00 0 00	7.7
	MOTA	4243	H2 H2O		18.739		4.084	1.00 0.00	W
	ATOM	4244	OH2 H2O		38.023	88.017	8.921	1.00 34.68	W
	ATOM	4245	н1 н20		37.201	88.224	9.366	1.00 0.00	W
_	MOTA	4246	H2 H2O		37.785	87.348	8.278	1.00 0.00	W
5	MOTA	4247	OH2 H2O		25.176	78.050	39.750	1.00 36.28	W
	ATOM	4248	H1 H2O	200	25.349	78.069	38.807	1.00 0.00	W
	MOTA	4249	H2 H2O	200	24.306	78.440	39.840	1.00 0.00	W
	MOTA	4250	он2 н2о		36.509		18.830	1.00 40.11	W
	MOTA	4251	H1 H2O		36.944	75.281	19.473	1.00 0.00	W
10	MOTA	4252	H2 H2O						
10					36.226	76.605	19.326	1.00 0.00	M
	ATOM	4253	он2 н2о	202	15.114	86.425	44.318	1.00 26.14	M
	ATOM	4254	н1 н2о		14.743	86.504	43.441	1.00 0.00	W
	ATOM	4255	H2 H2O	202	15.979	86.832	44.251	1.00 0.00	W
	ATOM	4256	он2 н2о	203	34.096	66.512	23.788	1.00 48.56	W
15	ATOM	4257	н1 н20		34.012	66.195	24.690	1.00 0.00	W
	ATOM	4258	H2 H2O		34.943	66.959	23.773	1.00 0.00	
	ATOM	4259	OH2 H2O		28.998				M
						83.540	37.915	1.00 48.28	M
	ATOM	4260	H1 H2O		29.160	83.028	37.122	1.00 0.00	M
• •	MOTA	4261	H2 H2O		29.874	83.729	38.257	1.00 0.00	M
20	MOTA	4262	OH2 H2O	205	36.771	86.241	17.583	1.00 28.64	W
	MOTA	4263	H1 H2O	205	37.720	86.287	17.698	1.00 0.00	W
	ATOM	4264	H2 H2O	205	36.608	86.681	16.750	1.00 0.00	W
	ATOM	4265	OH2 H2O	206	34.304	83.977	22.394		
								1.00 37.11	M
25	MOTA	4266	н1 н20	206	33.908	83.964	23.266	1.00 0.00	M
25	MOTA	4267	H2 H2O	206	33.588	84.238	21.812	1.00 0.00	W
	MOTA	4268	OH2 H2O	207	10.426	85.642	38.336	1.00 35.00	W
	ATOM	4269	H1 H2O	207	10.276	85.151	39.144	1.00 0.00	W
	ATOM	4270	H2 H2O	207	10.589	86.537	38.626	1.00 0.00	W
	ATOM	4271	ОН2 Н2О	208	33.164	40.493	36.564	1.00 43.55	W
30	ATOM	4272	H1 H2O	208	33.931	39.992	36.285		
50								1.00 0.00	W
	ATOM	4273	H2 H2O	208	32.453	40.170	36.012	1.00 0.00	W
	MOTA	4274	он2 н2о	209	9.667	59.806	49.799	1.00 27.66	W
	$\mathbf{MOTA}$	4275	н1 н20	209	9.078	59.514	49.107	1.00 0.00	W
	ATOM	4276	H2 H2O	209	10.523	59.452	49.554	1.00 0.00	W
35	ATOM	4277	OH2 H2O	210	40.620	91.683	9.844	1.00 44.74	W
	ATOM	4278	н1 н20	210	39.757	91.357	10.104	1.00 0.00	W
	ATOM	4279	H2 H2O	210	40.905	91.080	9.157	1.00 0.00	W
	ATOM	4280	OH2 H2O	211					
					31.114	53.143	38.106	1.00 19.43	W
40	MOTA	4281	н1 н20	211	30.669	52.292	38.079	1.00 0.00	W
40	ATOM	4282	H2 H2O	211	31.806	53.073	37.457	1.00 0.00	W
	ATOM	4283	он2 н2о	212	37.410	58.585	24.168	1.00 51.69	W
	ATOM	4284	H1 H2O	212	36.615	59.088	23.990	1.00 0.00	W
	ATOM	4285	H2 H2O	212	37.097	57.750	24.508	1.00 0.00	W
	MOTA	4286	ОН2 Н2О	213	37.530	82.337	17.584	1.00 25.73	W
45	ATOM	4287	H1 H2O	213	36.642	81.987	17.649	1.00 0.00	
15	ATOM	4288							W
			H2 H2O	213	38.090	81.564	17.520	1.00 0.00	W
	MOTA	4289	он2 н2о	214	20.562	62.057	49.243	1.00 36.13	W
	ATOM	4290	H1 H2O	214	20.191	62.888	48.941	1.00 0.00	W
	MOTA	4291	H2 H2O	214	20.159	61.398	48.677	1.00 0.00	W
50	MOTA	4292	OH2 H2O	215	38.487	67.744	46.984	1.00 28.08	W
	ATOM	4293	H1 H2O	215	38.487	68.698	46.981	1.00 0.00	W
	MOTA	4294	H2 H2O	215	38.487	67.501	46.054		
									W
	ATOM	4295	он2 н2о	216	4.672	50.241	43.410	1.00 37.85	W
	ATOM	4296	н1 н20	216	3.799	49.905	43.616	1.00 0.00	W
55	MOTA	4297	H2 H2O	216	5.068	50.420	44.262	1.00 0.00	W
	ATOM	4298	OH2 H2O	217	32.087	71.911	7.975	1.00 35.72	W
	MOTA	4299	H1 H2O	217	32.492	72.674	7.563	1.00 0.00	W
	MOTA	4300	H2 H2O	217	31.862	72.205	8.857	1.00 0.00	W
	ATOM	4301	OH2 H2O	218	37.077		31.371		
60						71.241		1.00 28.59	W
00	ATOM	4302	н1 н2о	218	36.181	71.414	31.087	1.00 0.00	W
	ATOM	4303	H2 H2O	218	37.354	70.488	30.847	1.00 0.00	W
	MOTA	4304	OH2 H2O	219	12.531	78.336	47.863	1.00 38.31	W
	MOTA	4305	H1 H2O	219	11.632	78.370	47.538	1.00 0.00	W
	ATOM	4306	H2 H2O	219	12.440	78.304	48.816	1.00 0.00	W
65	ATOM	4307	OH2 H2O	236	5.922	55.713	49.951	1.00 34.41	
55	ATOM	4307	H1 H20	236					W
					6.664	55.901	49.382	1.00 0.00	W
	ATOM	4309	H2 H2O	236	6.297	55.224	50.679	1.00 0.00	M
	MOTA	4310	он2 н2о	237	32.810	50.612	40.203	1.00 42.20	W
	MOTA	4311	н1 н20	237	32.021	51.115	40.399	1.00 0.00	W
70	MOTA	4312	H2 H2O	237	32.497	49.728	40.026	1.00 0.00	W
	ATOM	4313	OH2 H2O	238		101.122	-4.447	1.00 38.51	W
	MOTA	4314	H1 H20	238		101.299	-5.184	1.00 0.00	W
	ATOM	4315	H2 H2O	238		101.299			
	121 OII	<b>ユン</b> エフ	TIL MAU	230	10.7/4	100.2/0	-4.652	1.00 0.00	W

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5 AT AT AT AT AT	ATOM	4316		H20	239	17.874	69.091	56.692	1.00	38.94	W
	MOTA	4317	H1	H20	239	17.874	70.049	56.691	1.00	0.00	W
	ATOM	4318	H2	H20	239	17.874	68.852	55.764	1.00	0.00	W
	ATOM	4319	OH2	H20	240	12.249	77.436	-11.341	1.00	40.18	M
	MOTA	4320	H1	H20	240	12.960	78.076	-11.282	1.00	0.00	W
	ATOM	4321	H2	H20	240	12.370	77.023	-12.196	1.00	0.00	W
	MOTA	4322	OH2	H20	241	29.087	65.635	23.981	1.00	33.57	W
	ATOM	4323	H1	H20	241	28.790	65.725	24.885	1.00	0.00	W
	ATOM	4324	H2	H20	241	29.863	66.198	23.928	1.00	0.00	W